



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:35 AM UTC

PDB ID : 7VC0 / pdb_00007vc0
EMDB ID : EMD-31887
Title : Membrane arm of active state CI from Rotenone-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-09-01
Resolution : 2.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

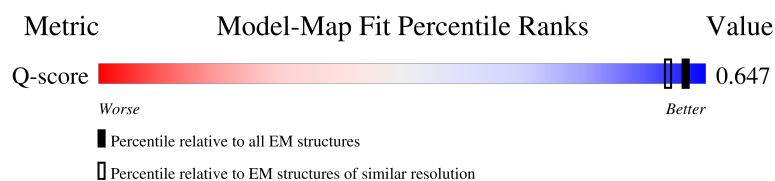
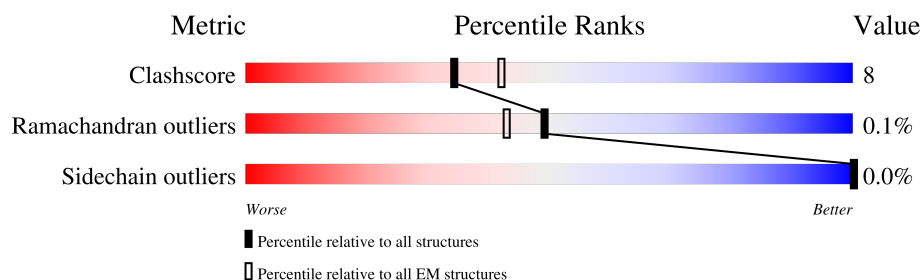
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Q	44	16% 77% 23%
2	S	70	87% 13%
3	U	83	8% 88% 12%
4	V	140	7% 88% 12%

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Mol	Chain	Length	Quality of chain
5	W	113	
6	X	88	
7	Y	67	
8	Z	80	
9	a	138	
10	b	126	
11	c	156	
12	d	175	
13	e	104	
14	f	49	
15	g	122	
16	h	105	
17	i	347	
18	j	115	
19	k	98	
20	l	606	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	125	
29	w	320	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 40048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	44	Total	C	N	O	S	0	0
			363	236	60	66	1		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			703	454	104	140	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	49	Total	C	N	O	0	0
			378	246	65	67		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	606	Total	C	N	O	S	0	0
			4807	3188	744	824	51		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	175	Total	C	N	O	S	0	0
			1298	867	188	230	13		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	125	Total	C	N	O	S	0	0
			1062	665	200	188	9		

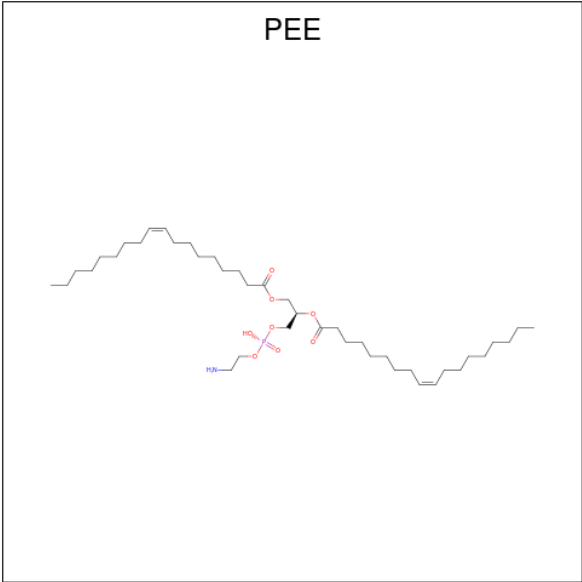
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

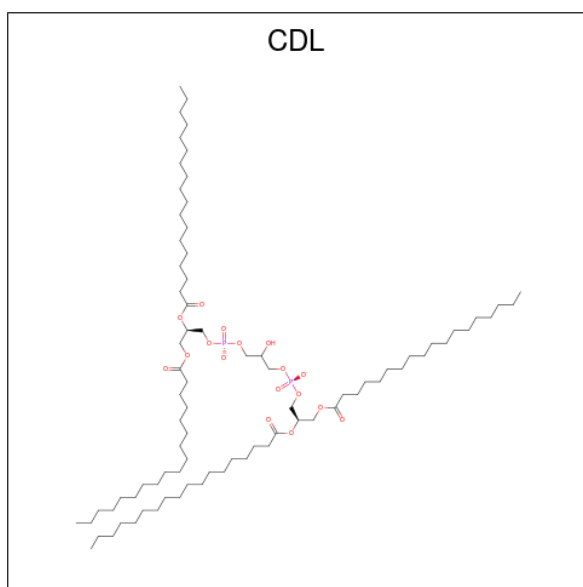
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



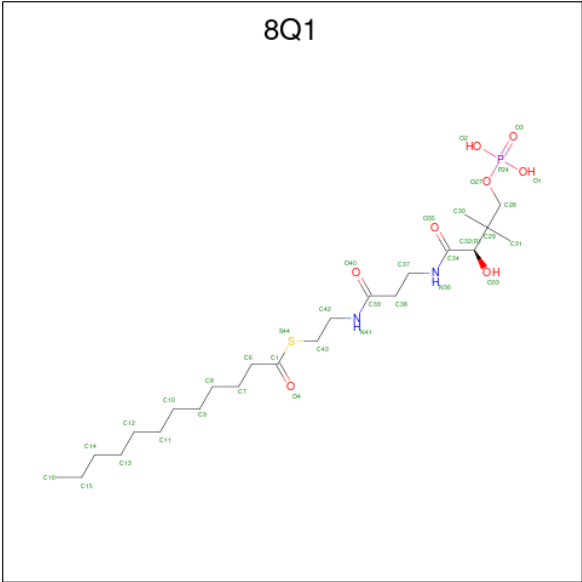
Mol	Chain	Residues	Atoms					AltConf
30	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	l	1	Total	C	N	O	P	0
			50	40	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



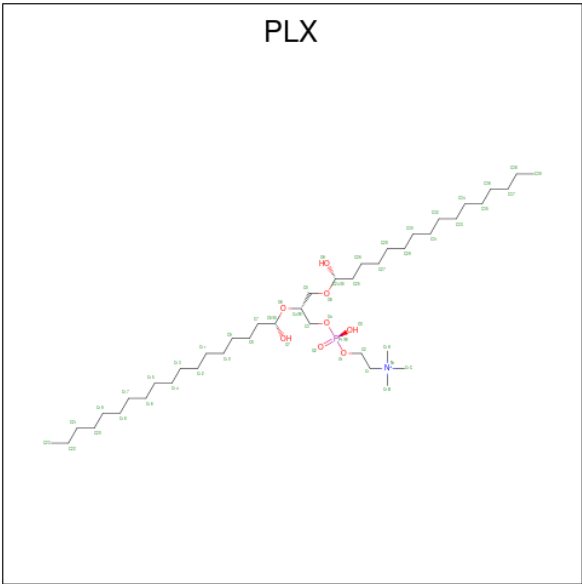
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	a	1	Total	C	O	P	0
			100	81	17	2	
31	k	1	Total	C	O	P	0
			100	81	17	2	
31	l	1	Total	C	O	P	0
			88	69	17	2	
31	o	1	Total	C	O	P	0
			100	81	17	2	
31	r	1	Total	C	O	P	0
			99	80	17	2	
31	r	1	Total	C	O	P	0
			76	57	17	2	
31	s	1	Total	C	O	P	0
			89	70	17	2	
31	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 32 is S-[2-(N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl)amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
32	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 33 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



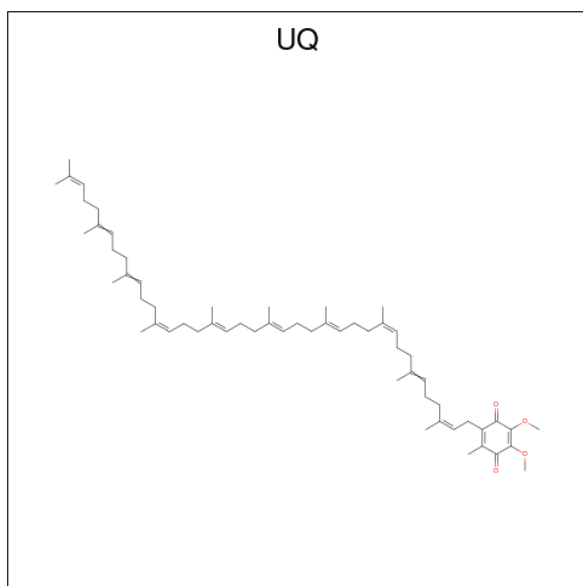
Mol	Chain	Residues	Atoms					AltConf
33	e	1	Total	C	N	O	P	0
			52	42	1	8	1	

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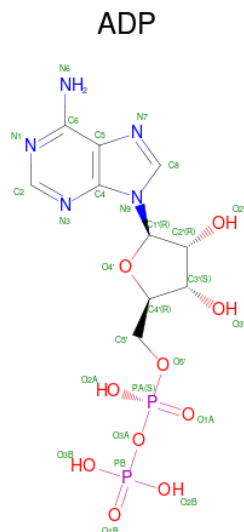
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	n	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			38	34	4	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	Q	5	Total O 5 5	0
36	S	5	Total O 5 5	0
36	U	3	Total O 3 3	0
36	V	2	Total O 2 2	0
36	W	2	Total O 2 2	0
36	Y	1	Total O 1 1	0
36	a	1	Total O 1 1	0
36	b	1	Total O 1 1	0
36	c	3	Total O 3 3	0
36	d	1	Total O 1 1	0
36	e	2	Total O 2 2	0

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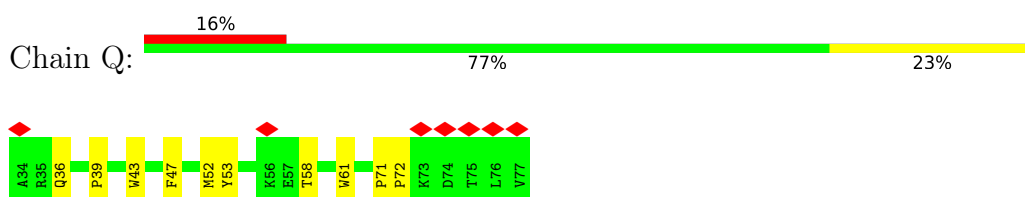
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Mol	Chain	Residues	Atoms		AltConf
36	h	5	Total 5	O 5	0
36	i	72	Total 72	O 72	0
36	j	27	Total 27	O 27	0
36	k	29	Total 29	O 29	0
36	l	63	Total 63	O 63	0
36	m	18	Total 18	O 18	0
36	n	2	Total 2	O 2	0
36	p	2	Total 2	O 2	0
36	r	85	Total 85	O 85	0
36	s	92	Total 92	O 92	0
36	u	1	Total 1	O 1	0
36	w	2	Total 2	O 2	0

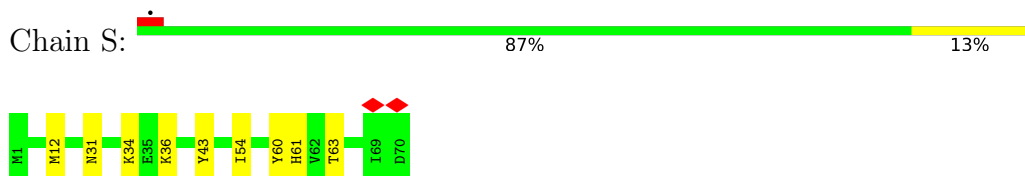
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

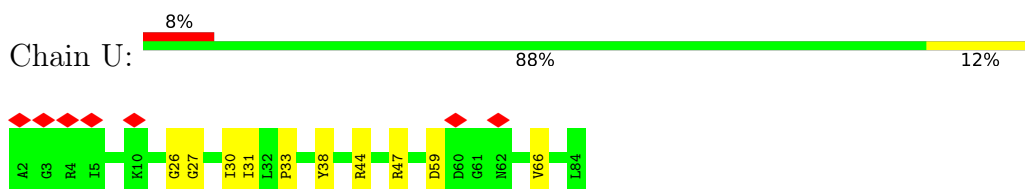
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



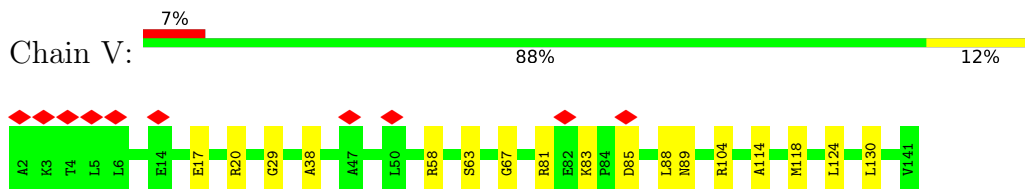
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



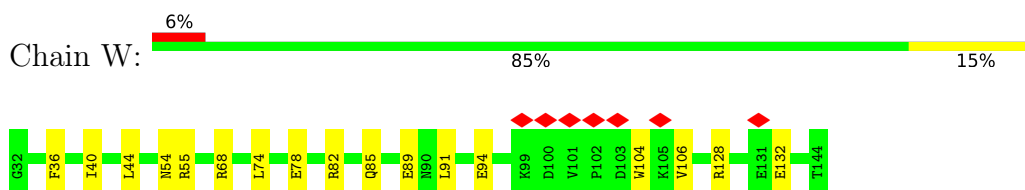
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



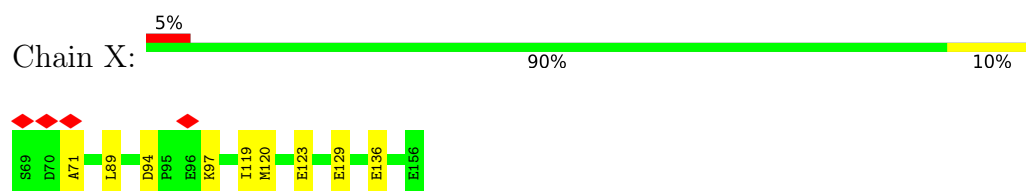
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



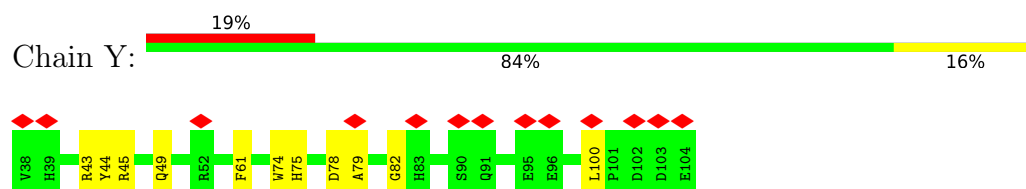
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



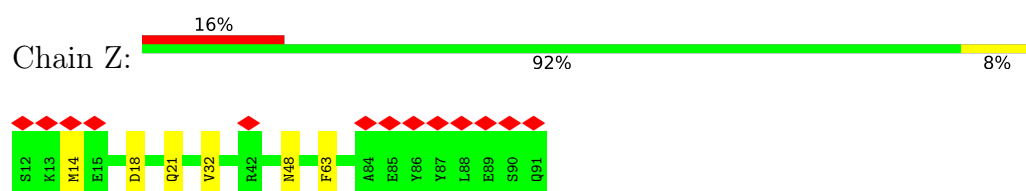
- Molecule 6: Acyl carrier protein, mitochondrial



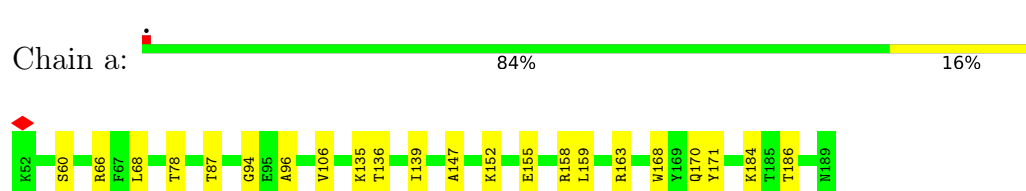
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



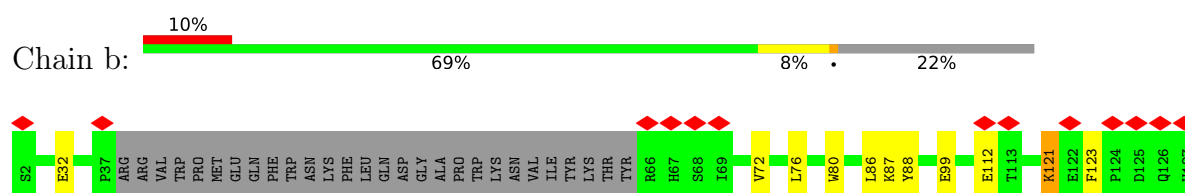
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



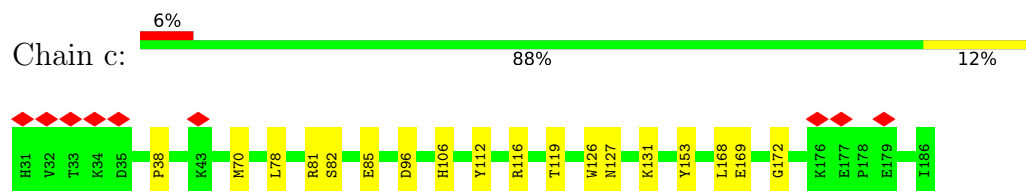
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



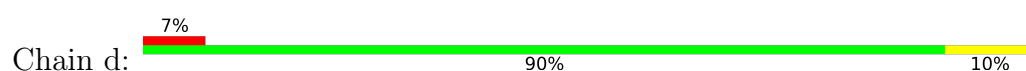
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

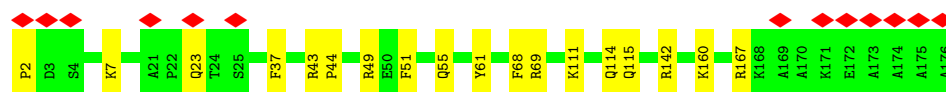


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

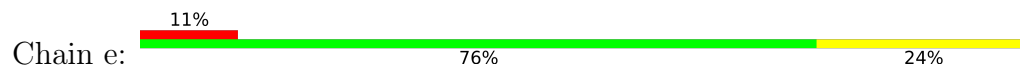


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10





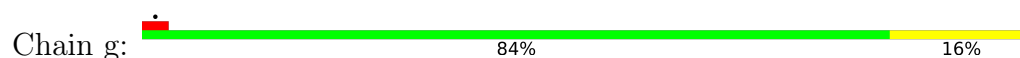
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



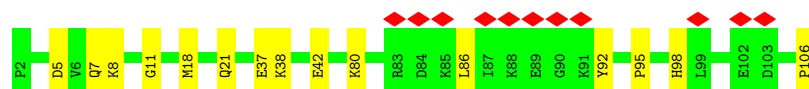
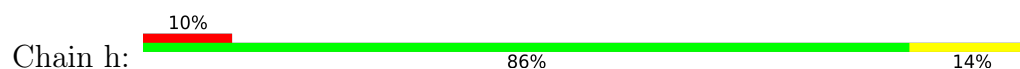
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



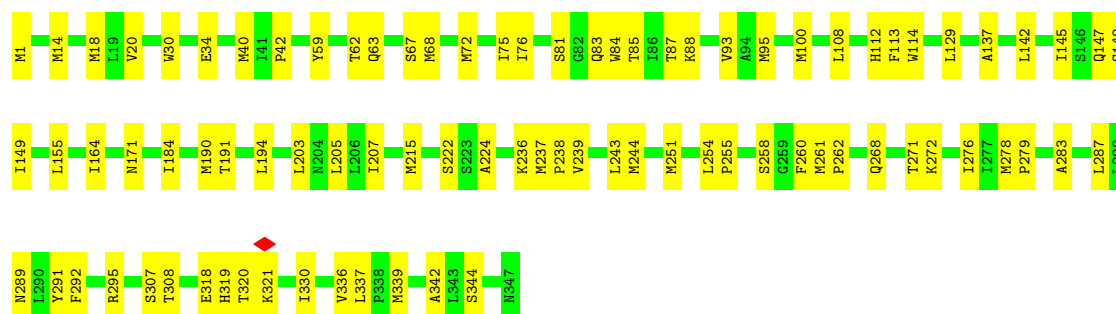
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

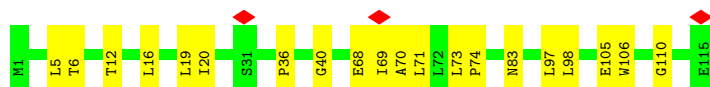


- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j:  83% 17%



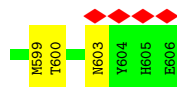
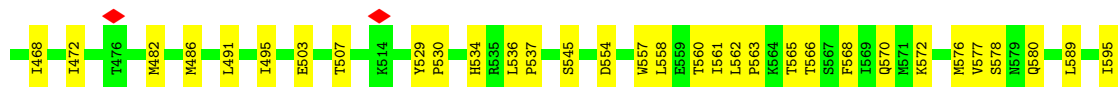
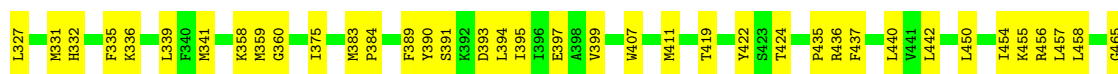
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  80% 20%



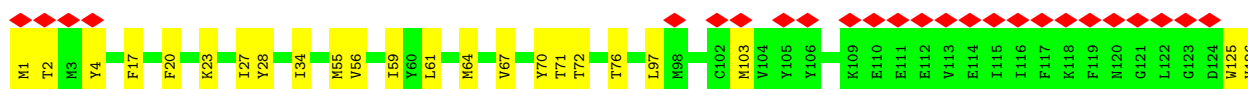
- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

Chain l:  76% 24%



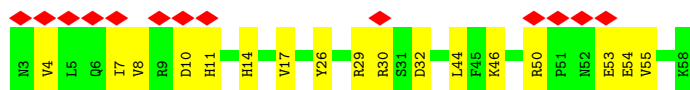
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m:  18% 84% 16%

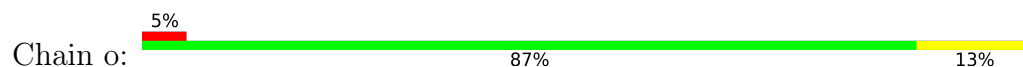


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

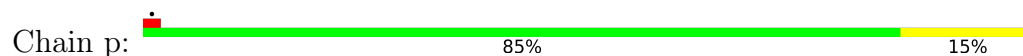
Chain n:  23% 70% 30%



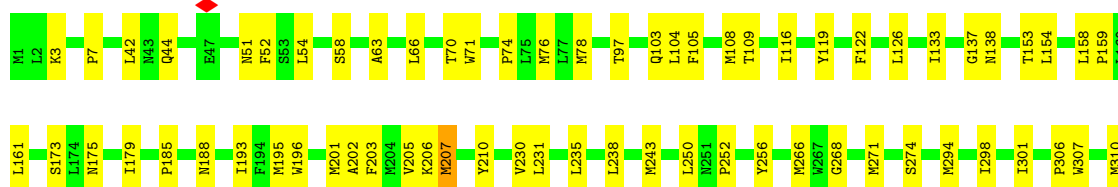
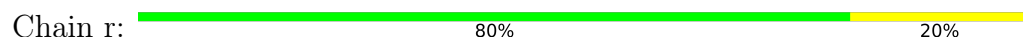
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



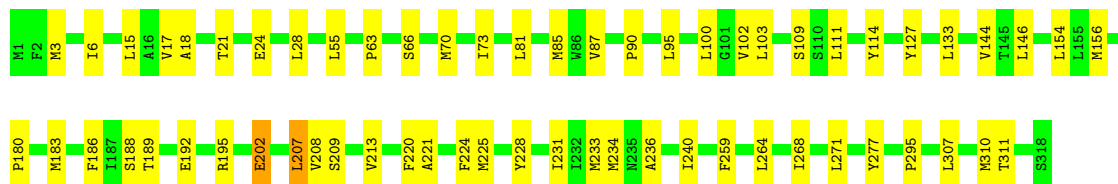
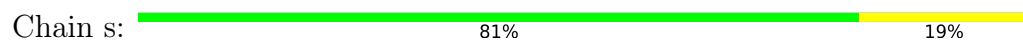
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



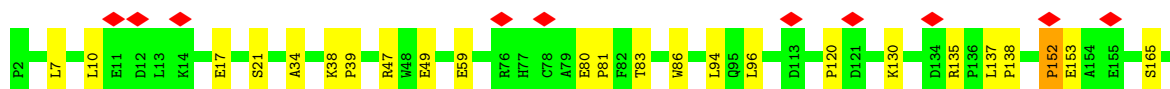
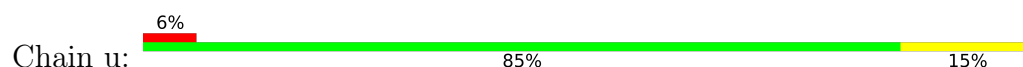
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4



- Molecule 26: NADH-ubiquinone oxidoreductase chain 1

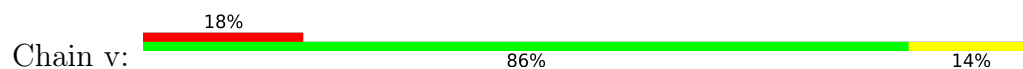


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

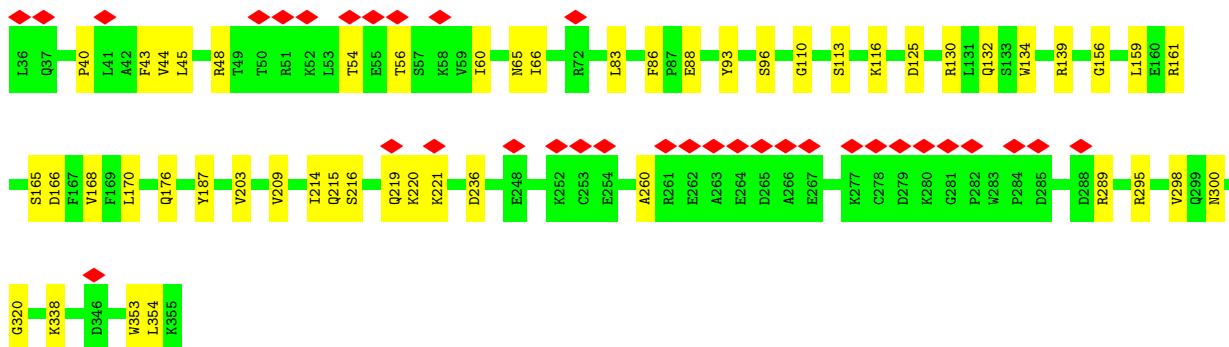
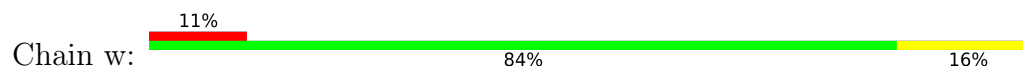




- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326044	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0152	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, 8Q1, CDL, UQ, PLX, ADP, PEE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Q	0.16	0/380	0.34	0/525
2	S	0.17	0/581	0.38	0/781
3	U	0.13	0/664	0.28	0/912
4	V	0.15	0/1042	0.31	0/1411
5	W	0.17	0/973	0.32	0/1312
6	X	0.15	0/715	0.35	0/967
7	Y	0.15	0/610	0.41	0/836
8	Z	0.12	0/660	0.30	0/892
9	a	0.17	0/1184	0.37	0/1603
10	b	0.18	0/844	0.45	1/1149 (0.1%)
11	c	0.17	0/1371	0.36	0/1875
12	d	0.17	0/1494	0.35	0/2015
13	e	0.16	0/891	0.34	0/1210
14	f	0.16	0/386	0.38	0/523
15	g	0.16	0/1036	0.34	0/1401
16	h	0.14	0/889	0.33	0/1190
17	i	0.21	0/2773	0.41	1/3768 (0.0%)
18	j	0.17	0/938	0.46	0/1281
19	k	0.21	0/759	0.44	0/1029
20	l	0.18	0/4937	0.39	0/6715
21	m	0.18	0/1331	0.40	0/1808
22	n	0.14	0/491	0.32	0/663
23	o	0.17	0/1092	0.38	0/1481
24	p	0.18	0/1590	0.39	0/2155
25	r	0.20	0/3723	0.42	0/5078
26	s	0.20	0/2581	0.42	0/3529
27	u	0.16	0/1436	0.37	0/1938
28	v	0.17	0/1071	0.39	0/1434
29	w	0.15	0/2650	0.38	0/3588
All	All	0.18	0/39092	0.39	2/53069 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	b	0	1
25	r	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	112	GLU	N-CA-C	5.14	116.88	111.28
17	i	113	PHE	N-CA-C	5.09	117.48	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	b	121	LYS	Peptide
25	r	207	MET	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	363	0	332	14	0
2	S	566	0	561	7	0
3	U	643	0	642	11	0
4	V	1021	0	1025	12	0
5	W	949	0	935	13	0
6	X	703	0	692	7	0
7	Y	584	0	529	8	0
8	Z	641	0	620	5	0
9	a	1151	0	1164	23	0
10	b	819	0	835	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	c	1315	0	1208	15	0
12	d	1461	0	1429	17	0
13	e	867	0	817	28	0
14	f	378	0	356	2	0
15	g	1005	0	999	22	0
16	h	867	0	871	15	0
17	i	2710	0	2874	72	0
18	j	914	0	951	16	0
19	k	748	0	799	24	0
20	l	4807	0	4946	104	0
21	m	1298	0	1272	26	0
22	n	479	0	486	15	0
23	o	1062	0	1072	16	0
24	p	1534	0	1470	20	0
25	r	3631	0	3839	81	0
26	s	2508	0	2607	50	0
27	u	1398	0	1374	22	0
28	v	1062	0	1036	14	0
29	w	2590	0	2553	39	0
30	Q	47	0	71	15	0
30	U	51	0	82	2	0
30	W	41	0	59	3	0
30	j	51	0	82	11	0
30	l	96	0	146	12	0
30	r	51	0	82	11	0
31	V	94	0	138	6	0
31	a	100	0	156	8	0
31	k	100	0	156	8	0
31	l	88	0	129	5	0
31	o	100	0	156	6	0
31	r	175	0	253	20	0
31	s	89	0	125	5	0
31	u	55	0	54	7	0
32	X	35	0	0	0	0
33	e	52	0	88	15	0
33	g	52	0	88	9	0
33	j	104	0	176	7	0
33	n	52	0	88	3	0
33	r	52	0	88	6	0
34	s	38	0	47	2	0
35	w	27	0	11	4	0
36	Q	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	S	5	0	0	0	0
36	U	3	0	0	0	0
36	V	2	0	0	0	0
36	W	2	0	0	0	0
36	Y	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	0	0
36	c	3	0	0	0	0
36	d	1	0	0	0	0
36	e	2	0	0	1	0
36	h	5	0	0	2	0
36	i	72	0	0	3	0
36	j	27	0	0	4	0
36	k	29	0	0	5	0
36	l	63	0	0	8	0
36	m	18	0	0	0	0
36	n	2	0	0	0	0
36	p	2	0	0	0	0
36	r	85	0	0	4	0
36	s	92	0	0	2	0
36	u	1	0	0	0	0
36	w	2	0	0	0	0
All	All	40048	0	40569	652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (652) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:201:MET:CE	30:r:501:PEE:H78	1.45	1.46
25:r:201:MET:HE2	30:r:501:PEE:C46	1.51	1.41
30:r:501:PEE:H33	30:r:501:PEE:H71	1.20	1.16
29:w:221:LYS:HE2	29:w:221:LYS:HA	1.27	1.14
25:r:122:PHE:CZ	25:r:206:LYS:CD	2.35	1.08
3:U:30:ILE:HD12	30:j:201:PEE:H43	1.37	1.06
25:r:122:PHE:CZ	25:r:206:LYS:HD2	1.93	1.01
29:w:139:ARG:HH12	35:w:401:ADP:N6	1.60	0.99
30:Q:101:PEE:H37	30:Q:101:PEE:C37	1.94	0.98
25:r:122:PHE:HZ	25:r:206:LYS:HD3	1.31	0.96
1:Q:53:TYR:CE1	30:Q:101:PEE:H2	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:101:PEE:H42	30:Q:101:PEE:H34	1.48	0.94
17:i:268:GLN:HE22	17:i:272:LYS:HE3	1.34	0.93
25:r:122:PHE:CZ	25:r:206:LYS:HD3	2.00	0.92
25:r:122:PHE:HZ	25:r:206:LYS:CD	1.79	0.91
30:r:501:PEE:H33	30:r:501:PEE:C42	2.01	0.90
29:w:139:ARG:HH12	35:w:401:ADP:HN61	0.91	0.88
29:w:139:ARG:NH1	35:w:401:ADP:HN61	1.72	0.88
36:l:825:HOH:O	25:r:400:MET:HE3	1.75	0.87
30:Q:101:PEE:H37	30:Q:101:PEE:H60	1.57	0.86
29:w:216:SER:O	29:w:220:LYS:HG3	1.75	0.85
20:l:491:LEU:O	20:l:495:ILE:HG12	1.78	0.83
13:e:103:SER:OG	33:e:201:PLX:H282	1.79	0.83
19:k:37:MET:HE1	19:k:63:LEU:HG	1.61	0.83
20:l:252:MET:SD	36:l:860:HOH:O	2.38	0.80
17:i:236:LYS:HG3	17:i:237:MET:HG3	1.63	0.79
3:U:26:GLY:HA3	30:j:201:PEE:H37	1.63	0.79
33:e:201:PLX:H21	30:l:703:PEE:H2	1.65	0.78
17:i:268:GLN:HG3	27:u:168:PHE:HZ	1.48	0.78
20:l:2:ASN:ND2	20:l:59:GLN:OE1	2.16	0.77
33:e:201:PLX:H6	25:r:449:LEU:HD13	1.64	0.77
1:Q:53:TYR:CE1	30:Q:101:PEE:C1	2.67	0.77
17:i:68:MET:CE	36:k:202:HOH:O	2.32	0.77
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.66	0.77
20:l:580:GLN:OE1	36:l:801:HOH:O	2.02	0.77
17:i:289:ASN:ND2	36:i:401:HOH:O	2.19	0.75
20:l:176:ARG:HG2	25:r:401:MET:HA	1.68	0.75
19:k:64:LEU:HD23	36:k:229:HOH:O	1.86	0.75
33:e:201:PLX:C14	31:r:503:CDL:H802	2.16	0.75
1:Q:53:TYR:HE1	30:Q:101:PEE:C1	2.00	0.75
31:r:504:CDL:O1	29:w:338:LYS:NZ	2.20	0.74
29:w:221:LYS:HE2	29:w:221:LYS:CA	2.12	0.74
25:r:387:SER:HB3	36:r:627:HOH:O	1.87	0.74
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.69	0.74
18:j:83:ASN:HA	36:j:319:HOH:O	1.88	0.74
17:i:258:SER:OG	17:i:336:VAL:HG22	1.88	0.73
31:a:201:CDL:H111	30:l:703:PEE:H60	1.70	0.73
1:Q:53:TYR:HE1	30:Q:101:PEE:H2	1.54	0.72
26:s:6:ILE:HD13	26:s:95:LEU:HD21	1.71	0.72
31:u:201:CDL:H581	31:u:201:CDL:H541	1.72	0.72
9:a:78:THR:HG21	13:e:96:SER:HA	1.72	0.72
23:o:20:PRO:HA	24:p:65:ARG:HH12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:72:THR:HG21	26:s:133:LEU:HD21	1.73	0.71
17:i:207:ILE:HD13	17:i:262:PRO:HD3	1.72	0.70
31:V:201:CDL:H521	20:l:577:VAL:HA	1.72	0.70
25:r:159:PRO:HB3	30:r:501:PEE:H25	1.73	0.70
20:l:599:MET:SD	20:l:603:ASN:ND2	2.64	0.70
3:U:30:ILE:CD1	30:j:201:PEE:H43	2.19	0.70
1:Q:53:TYR:CZ	30:Q:101:PEE:H2	2.25	0.70
16:h:37:GLU:OE1	36:h:201:HOH:O	2.08	0.70
29:w:125:ASP:O	29:w:130:ARG:NH2	2.25	0.70
25:r:203:PHE:O	25:r:207:MET:HG2	1.93	0.69
16:h:5:ASP:OD2	16:h:8:LYS:HB3	1.91	0.69
17:i:237:MET:SD	17:i:319:HIS:NE2	2.64	0.69
19:k:13:ALA:HB1	31:k:101:CDL:H821	1.74	0.69
17:i:88:LYS:HG3	17:i:148:SER:HB2	1.75	0.68
29:w:113:SER:HB3	29:w:116:LYS:HG2	1.75	0.68
30:Q:101:PEE:H37	30:Q:101:PEE:C36	2.23	0.68
5:W:82:ARG:NH1	16:h:106:PRO:O	2.27	0.68
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.75	0.68
6:X:94:ASP:HB3	6:X:97:LYS:HG2	1.75	0.68
20:l:227:PHE:O	20:l:230:HIS:ND1	2.27	0.67
20:l:393:ASP:OD1	36:l:802:HOH:O	2.13	0.67
5:W:36:PHE:O	5:W:40:ILE:HG12	1.95	0.67
15:g:3:MET:HG2	15:g:4:MET:HG3	1.77	0.67
25:r:78:MET:HE1	25:r:439:LEU:HD12	1.77	0.67
3:U:26:GLY:HA3	30:j:201:PEE:C23	2.24	0.67
5:W:94:GLU:OE2	5:W:104:TRP:NE1	2.28	0.66
25:r:370:PRO:HG3	25:r:375:LEU:HD13	1.77	0.66
20:l:170:GLN:NE2	30:l:702:PEE:O1P	2.28	0.66
24:p:127:ARG:NH1	24:p:131:GLU:OE1	2.29	0.66
4:V:81:ARG:HH12	4:V:88:LEU:HD23	1.60	0.66
19:k:37:MET:HE2	19:k:67:ALA:HB2	1.77	0.66
17:i:68:MET:HE3	36:k:202:HOH:O	1.95	0.66
26:s:18:ALA:O	26:s:21:THR:OG1	2.14	0.65
20:l:390:TYR:O	20:l:394:LEU:HD12	1.95	0.65
26:s:207:LEU:O	26:s:209:SER:N	2.29	0.65
18:j:36:PRO:O	36:j:301:HOH:O	2.15	0.65
20:l:66:TRP:CD1	30:l:703:PEE:H16	2.32	0.65
9:a:106:VAL:HG13	22:n:50:ARG:HH21	1.60	0.65
31:u:201:CDL:H581	31:u:201:CDL:C54	2.27	0.64
9:a:159:LEU:HD22	9:a:163:ARG:HH12	1.62	0.64
29:w:221:LYS:HA	29:w:221:LYS:CE	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:31:ASN:OD1	2:S:60:TYR:OH	2.12	0.63
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.80	0.63
22:n:29:ARG:NH2	33:n:101:PLX:O3	2.31	0.63
3:U:44:ARG:HG2	3:U:47:ARG:HH21	1.64	0.63
24:p:47:ARG:NH2	24:p:70:GLU:OE1	2.31	0.63
15:g:35:TYR:CE1	31:u:201:CDL:H771	2.34	0.63
20:l:286:LEU:HD13	20:l:411:MET:SD	2.39	0.63
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.30	0.63
26:s:146:LEU:HD12	26:s:188:SER:HB3	1.80	0.62
12:d:160:LYS:NZ	15:g:114:ILE:O	2.32	0.62
25:r:122:PHE:HE1	25:r:238:LEU:HB3	1.63	0.62
33:e:201:PLX:H1A2	33:e:201:PLX:O1	1.99	0.62
28:v:17:PRO:HB3	28:v:105:GLU:OE1	2.00	0.62
26:s:220:PHE:CE1	26:s:224:PHE:HE2	2.17	0.62
12:d:2:PRO:O	12:d:7:LYS:NZ	2.33	0.61
21:m:27:ILE:HG22	26:s:70:MET:HE1	1.83	0.61
17:i:268:GLN:NE2	17:i:272:LYS:HE3	2.12	0.61
30:j:201:PEE:H26	26:s:295:PRO:HB3	1.83	0.61
25:r:44:GLN:OE1	36:r:601:HOH:O	2.16	0.61
18:j:68:GLU:HG3	18:j:98:LEU:HD13	1.82	0.61
15:g:35:TYR:HE1	31:u:201:CDL:H771	1.65	0.61
30:j:201:PEE:O5	30:j:201:PEE:H55	2.00	0.61
20:l:228:GLY:HA3	30:l:702:PEE:H38	1.83	0.60
16:h:18:MET:HE3	19:k:56:ALA:HA	1.83	0.60
20:l:190:LEU:HD11	25:r:307:TRP:CH2	2.36	0.60
5:W:74:LEU:O	5:W:78:GLU:HG3	2.01	0.60
12:d:23:GLN:HB2	28:v:72:ASP:HB3	1.82	0.60
33:g:201:PLX:H332	17:i:342:ALA:HB3	1.82	0.60
25:r:122:PHE:CE2	25:r:206:LYS:HD2	2.35	0.60
4:V:81:ARG:NH1	4:V:88:LEU:HD23	2.16	0.60
4:V:124:LEU:HD11	30:r:501:PEE:H64	1.84	0.60
19:k:27:MET:HE1	21:m:70:TYR:HB3	1.82	0.60
25:r:188:ASN:OD1	25:r:256:TYR:OH	2.15	0.60
25:r:243:MET:HB3	25:r:301:ILE:HG21	1.83	0.60
20:l:27:TYR:O	20:l:115:ASN:ND2	2.33	0.59
20:l:249:SER:HB2	20:l:336:LYS:HG3	1.83	0.59
12:d:167:ARG:HH21	13:e:153:GLU:HG3	1.67	0.59
20:l:419:THR:HA	20:l:422:TYR:CE2	2.38	0.59
25:r:104:LEU:HG	25:r:108:MET:HE2	1.85	0.59
11:c:168:LEU:HA	11:c:172:GLY:HA2	1.85	0.59
17:i:93:VAL:HA	20:l:603:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:32:GLU:HB3	24:p:115:TYR:HD1	1.66	0.59
4:V:114:ALA:HB1	4:V:118:MET:HE3	1.85	0.59
12:d:114:GLN:HG3	20:l:203:MET:HG2	1.85	0.59
20:l:545:SER:OG	25:r:274:SER:O	2.21	0.59
1:Q:53:TYR:OH	30:Q:101:PEE:H2	2.03	0.58
22:n:26:TYR:OH	22:n:30:ARG:NH1	2.35	0.58
22:n:50:ARG:HB2	22:n:53:GLU:HG2	1.85	0.58
17:i:88:LYS:HB2	17:i:147:GLN:HE21	1.68	0.58
25:r:195:MET:HA	30:r:501:PEE:H16	1.84	0.58
17:i:42:PRO:HG3	21:m:167:VAL:HG13	1.84	0.58
25:r:306:PRO:HB3	25:r:458:LEU:HD12	1.85	0.58
1:Q:47:PHE:HD1	1:Q:52:MET:HE1	1.69	0.58
20:l:596:MET:O	20:l:600:THR:HG23	2.03	0.58
33:e:201:PLX:C15	31:r:503:CDL:H802	2.33	0.58
21:m:61:LEU:O	26:s:114:TYR:OH	2.21	0.58
20:l:359:MET:O	20:l:436:ARG:NH2	2.37	0.57
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.85	0.57
29:w:295:ARG:HA	29:w:298:VAL:HG22	1.84	0.57
25:r:335:GLU:OE1	36:r:602:HOH:O	2.17	0.57
25:r:201:MET:CE	30:r:501:PEE:C46	2.39	0.57
23:o:28:GLU:HA	23:o:31:LYS:HG2	1.87	0.57
29:w:209:VAL:HG22	29:w:260:ALA:HB2	1.86	0.57
12:d:69:ARG:NH2	22:n:46:LYS:O	2.38	0.56
20:l:450:LEU:O	20:l:454:ILE:HG12	2.05	0.56
31:k:101:CDL:H571	31:k:101:CDL:H761	1.87	0.56
11:c:116:ARG:HG2	30:l:702:PEE:H49	1.87	0.56
17:i:30:TRP:O	17:i:34:GLU:HG2	2.04	0.56
19:k:31:LEU:HD21	21:m:67:VAL:HG11	1.87	0.56
20:l:257:VAL:HG13	20:l:317:ILE:HD11	1.86	0.56
25:r:201:MET:HE1	33:r:502:PLX:H201	1.88	0.56
17:i:238:PRO:HB2	31:r:504:CDL:HA32	1.86	0.56
20:l:558:LEU:HD21	31:o:201:CDL:H871	1.88	0.56
26:s:109:SER:OG	26:s:192:GLU:OE2	2.22	0.56
36:j:317:HOH:O	21:m:59:ILE:HD13	2.05	0.56
19:k:10:MET:HE2	21:m:103:MET:SD	2.46	0.56
25:r:202:ALA:O	25:r:205:VAL:HG12	2.05	0.56
13:e:105:PHE:HB2	33:n:101:PLX:H141	1.88	0.56
15:g:13:LEU:HA	33:g:201:PLX:H32	1.88	0.55
25:r:105:PHE:O	25:r:109:THR:OG1	2.24	0.55
30:Q:101:PEE:H37	30:Q:101:PEE:H59	1.87	0.55
21:m:1:MET:HB2	21:m:125:TRP:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:21:GLN:HA	19:k:53:PHE:CE1	2.42	0.55
19:k:65:VAL:HG11	21:m:157:THR:HG23	1.87	0.55
20:l:51:LEU:HG	20:l:55:MET:HE2	1.89	0.55
19:k:30:LEU:HD13	36:k:223:HOH:O	2.07	0.55
20:l:397:GLU:HG2	20:l:482:MET:HE1	1.90	0.54
18:j:71:LEU:O	21:m:147:TYR:OH	2.19	0.54
33:e:201:PLX:H151	31:r:503:CDL:H802	1.88	0.54
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.90	0.54
9:a:66:ARG:HH12	13:e:72:ASP:HB2	1.72	0.54
20:l:11:THR:HG21	20:l:47:SER:HB3	1.89	0.54
4:V:85:ASP:HB3	4:V:130:LEU:HD21	1.90	0.54
15:g:36:MET:HE1	33:g:201:PLX:H393	1.90	0.54
20:l:503:GLU:O	20:l:507:THR:HG23	2.08	0.54
29:w:60:ILE:HG12	29:w:203:VAL:HB	1.89	0.54
20:l:71:LEU:HD12	25:r:310:MET:HE1	1.90	0.54
25:r:133:ILE:HD11	25:r:231:LEU:HD11	1.90	0.54
33:e:201:PLX:C2	30:l:703:PEE:H2	2.38	0.54
20:l:286:LEU:HD21	31:l:701:CDL:H812	1.89	0.53
3:U:30:ILE:HD12	30:j:201:PEE:C26	2.25	0.53
11:c:81:ARG:NH1	11:c:85:GLU:OE2	2.38	0.53
11:c:70:MET:HE2	23:o:85:LYS:HZ2	1.74	0.53
27:u:169:PHE:CE1	31:u:201:CDL:H561	2.43	0.53
25:r:403:THR:HA	25:r:406:TYR:CE2	2.43	0.53
17:i:171:ASN:ND2	20:l:578:SER:OG	2.32	0.53
20:l:223:LYS:NZ	36:l:809:HOH:O	2.38	0.53
25:r:201:MET:HE2	30:r:501:PEE:C45	2.34	0.53
7:Y:74:TRP:HD1	7:Y:75:HIS:CE1	2.27	0.53
20:l:136:ASN:HA	20:l:197:ASP:HA	1.91	0.53
25:r:343:ILE:O	25:r:346:ARG:NH1	2.36	0.53
11:c:70:MET:HE2	23:o:85:LYS:NZ	2.24	0.52
17:i:84:TRP:CH2	19:k:59:MET:HE3	2.44	0.52
18:j:69:ILE:HD11	26:s:144:VAL:HA	1.91	0.52
26:s:24:GLU:OE1	26:s:228:TYR:OH	2.16	0.52
33:e:201:PLX:H141	31:r:503:CDL:H802	1.91	0.52
25:r:122:PHE:CE1	25:r:238:LEU:HB3	2.44	0.52
5:W:54:ASN:ND2	26:s:156:MET:SD	2.82	0.52
17:i:68:MET:HE1	19:k:37:MET:SD	2.49	0.52
20:l:179:ASP:HB3	36:l:825:HOH:O	2.09	0.52
25:r:202:ALA:O	25:r:205:VAL:CG1	2.56	0.52
23:o:95:ILE:HD11	31:o:201:CDL:H802	1.92	0.52
20:l:294:THR:HG22	31:l:701:CDL:HB62	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:11:HIS:HD2	22:n:14:HIS:CE1	2.27	0.52
29:w:86:PHE:HB2	29:w:159:LEU:HD23	1.92	0.52
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.44	0.52
20:l:97:THR:HG21	20:l:125:LEU:HD22	1.91	0.52
25:r:175:ASN:O	25:r:179:ILE:HG12	2.10	0.52
31:u:201:CDL:H772	31:u:201:CDL:H731	1.92	0.52
17:i:222:SER:O	17:i:224:ALA:N	2.42	0.52
30:Q:101:PEE:H42	30:Q:101:PEE:C21	2.28	0.51
31:r:503:CDL:HB21	31:r:503:CDL:HB62	1.91	0.51
26:s:73:ILE:HD11	31:s:401:CDL:H172	1.92	0.51
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.92	0.51
9:a:159:LEU:HD22	9:a:163:ARG:NH1	2.26	0.51
11:c:38:PRO:HG2	23:o:70:TYR:HD2	1.75	0.51
20:l:554:ASP:OD1	36:l:803:HOH:O	2.18	0.51
20:l:566:THR:O	20:l:570:GLN:HG2	2.10	0.51
31:V:201:CDL:H612	31:V:201:CDL:H752	1.93	0.51
10:b:32:GLU:OE2	24:p:117:ASP:HB2	2.10	0.51
24:p:28:GLU:OE2	24:p:34:ARG:NH1	2.41	0.51
25:r:373:ILE:HD11	25:r:444:LEU:HD12	1.93	0.51
20:l:316:THR:HG23	20:l:325:ALA:HB2	1.91	0.51
25:r:207:MET:HE2	25:r:298:ILE:HG13	1.93	0.51
30:r:501:PEE:H33	30:r:501:PEE:C43	2.40	0.51
33:e:201:PLX:H122	31:r:503:CDL:H632	1.93	0.51
19:k:17:ALA:HB2	31:k:101:CDL:H812	1.93	0.51
20:l:141:PHE:HE2	25:r:375:LEU:HD11	1.75	0.51
20:l:530:PRO:O	20:l:534:HIS:HB2	2.11	0.51
26:s:55:LEU:HD13	26:s:221:ALA:HB2	1.91	0.51
30:U:401:PEE:H59	26:s:277:TYR:HE2	1.76	0.51
4:V:58:ARG:HG3	4:V:104:ARG:NH2	2.26	0.51
17:i:203:LEU:HD11	17:i:261:MET:HE3	1.92	0.51
23:o:31:LYS:O	23:o:35:GLU:HG3	2.11	0.51
17:i:100:MET:HE1	20:l:595:ILE:HG23	1.91	0.51
17:i:283:ALA:HB1	25:r:158:LEU:HD22	1.92	0.51
20:l:331:MET:SD	20:l:465:GLY:HA2	2.50	0.51
4:V:17:GLU:OE1	4:V:20:ARG:NH1	2.40	0.51
25:r:372:SER:HB3	31:r:503:CDL:H381	1.93	0.51
26:s:73:ILE:HD13	31:s:401:CDL:H551	1.93	0.51
21:m:17:PHE:HA	21:m:20:PHE:CE2	2.46	0.51
28:v:29:TYR:OH	28:v:111:ARG:NH2	2.44	0.51
25:r:193:ILE:HD13	33:r:502:PLX:H102	1.92	0.50
31:u:201:CDL:H772	31:u:201:CDL:C73	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:57:GLU:OE1	29:w:320:GLY:HA3	2.11	0.50
21:m:28:TYR:CE1	26:s:70:MET:HE3	2.46	0.50
9:a:155:GLU:OE2	9:a:158:ARG:NH2	2.40	0.50
20:l:339:LEU:HD13	36:l:863:HOH:O	2.10	0.50
26:s:63:PRO:HB2	26:s:66:SER:HB3	1.93	0.50
17:i:84:TRP:HH2	19:k:59:MET:HE3	1.76	0.50
17:i:155:LEU:HD22	17:i:278:MET:HE2	1.93	0.50
5:W:40:ILE:O	5:W:44:LEU:HG	2.12	0.50
6:X:119:ILE:O	6:X:123:GLU:HG3	2.11	0.50
8:Z:14:MET:HE1	20:l:440:LEU:HD11	1.93	0.50
12:d:115:GLN:HG2	20:l:62:ILE:HG12	1.94	0.50
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.93	0.50
18:j:16:LEU:HD13	18:j:19:LEU:HD12	1.93	0.50
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.92	0.50
17:i:81:SER:O	17:i:83:GLN:N	2.38	0.50
17:i:112:HIS:HB2	17:i:184:ILE:HD13	1.93	0.50
20:l:341:MET:CE	20:l:457:LEU:HD12	2.42	0.50
3:U:38:TYR:HB2	26:s:310:MET:O	2.12	0.50
12:d:68:PHE:HD1	22:n:44:LEU:HD11	1.77	0.50
16:h:21:GLN:HB2	36:h:201:HOH:O	2.11	0.49
17:i:239:VAL:HG22	31:r:504:CDL:HA62	1.93	0.49
22:n:10:ASP:OD1	22:n:11:HIS:ND1	2.45	0.49
13:e:72:ASP:OD1	13:e:72:ASP:N	2.43	0.49
25:r:70:THR:HA	25:r:103:GLN:NE2	2.27	0.49
26:s:127:TYR:HD1	26:s:207:LEU:HB3	1.78	0.49
10:b:99:GLU:HG2	20:l:61:MET:HG3	1.94	0.49
4:V:81:ARG:HE	4:V:83:LYS:HB2	1.77	0.49
6:X:120:MET:HE1	24:p:24:LEU:HB3	1.93	0.49
28:v:22:MET:HE1	28:v:102:PHE:HA	1.94	0.49
30:Q:101:PEE:O1P	17:i:291:TYR:OH	2.23	0.49
3:U:27:GLY:O	3:U:31:ILE:HG12	2.13	0.49
17:i:295:ARG:NH1	36:i:414:HOH:O	2.46	0.49
25:r:207:MET:O	25:r:294:MET:HG3	2.12	0.49
26:s:202:GLU:HB2	36:s:557:HOH:O	2.13	0.49
29:w:139:ARG:NH1	35:w:401:ADP:N6	2.42	0.49
29:w:215:GLN:O	29:w:219:GLN:HG2	2.13	0.49
31:a:201:CDL:H212	31:a:201:CDL:H761	1.95	0.49
17:i:215:MET:HG3	17:i:251:MET:SD	2.53	0.49
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.48	0.49
5:W:91:LEU:HD22	27:u:7:LEU:HD12	1.94	0.49
31:a:201:CDL:H362	10:b:80:TRP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:201:CDL:H772	13:e:100:VAL:HG22	1.95	0.49
10:b:72:VAL:HG23	10:b:76:LEU:HD23	1.95	0.48
19:k:4:VAL:O	19:k:8:ILE:HG12	2.13	0.48
21:m:126:VAL:HG23	21:m:127:ILE:HG23	1.95	0.48
28:v:116:GLU:O	28:v:119:GLU:HG3	2.14	0.48
20:l:341:MET:HE2	20:l:457:LEU:HD12	1.95	0.48
24:p:98:LYS:HG2	24:p:178:PRO:HG3	1.95	0.48
27:u:94:LEU:HD23	27:u:96:LEU:HD21	1.93	0.48
2:S:63:THR:HG23	27:u:21:SER:HB2	1.94	0.48
29:w:353:TRP:H	29:w:353:TRP:CD1	2.31	0.48
4:V:29:GLY:O	4:V:63:SER:OG	2.26	0.48
20:l:486:MET:HE2	28:v:1:MYR:H51	1.96	0.48
26:s:156:MET:HE2	36:s:569:HOH:O	2.14	0.48
23:o:56:ARG:NH1	25:r:422:HIS:O	2.29	0.48
26:s:228:TYR:HA	26:s:231:ILE:HD12	1.95	0.48
15:g:45:LEU:HB3	31:r:504:CDL:H731	1.96	0.48
27:u:83:THR:HA	27:u:86:TRP:CD1	2.48	0.48
2:S:54:ILE:HD11	27:u:21:SER:HA	1.95	0.48
17:i:207:ILE:HD11	17:i:261:MET:HE3	1.95	0.48
33:j:203:PLX:H311	33:j:203:PLX:H282	1.61	0.48
13:e:92:PHE:O	13:e:96:SER:HB2	2.14	0.47
17:i:190:MET:HE2	17:i:205:LEU:HA	1.95	0.47
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.49	0.47
23:o:116:ILE:HG12	23:o:121:LEU:HD22	1.96	0.47
31:V:201:CDL:H322	20:l:576:MET:HE1	1.96	0.47
19:k:33:LEU:HG	36:k:201:HOH:O	2.14	0.47
20:l:375:ILE:HD12	20:l:458:LEU:HD11	1.96	0.47
21:m:71:THR:O	21:m:76:THR:HG23	2.14	0.47
26:s:236:ALA:HB1	26:s:259:PHE:HZ	1.78	0.47
21:m:97:LEU:HD11	31:s:401:CDL:H422	1.95	0.47
31:k:101:CDL:H782	31:k:101:CDL:H592	1.96	0.47
25:r:42:LEU:HB3	25:r:453:MET:CE	2.45	0.47
25:r:126:LEU:HD21	25:r:153:THR:HG21	1.96	0.47
15:g:52:ARG:NH1	17:i:318:GLU:OE2	2.48	0.47
20:l:245:ALA:O	20:l:249:SER:OG	2.31	0.47
22:n:17:VAL:HG13	25:r:7:PRO:HB3	1.96	0.47
24:p:19:LEU:HD13	24:p:68:GLU:OE2	2.14	0.47
25:r:97:THR:HG21	31:r:504:CDL:H241	1.97	0.47
1:Q:36:GLN:NE2	25:r:137:GLY:O	2.48	0.47
17:i:254:LEU:HD21	25:r:154:LEU:HD11	1.97	0.47
20:l:95:PHE:CZ	20:l:456:ARG:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:368:ALA:O	25:r:375:LEU:HD12	2.14	0.47
26:s:15:LEU:HD12	34:s:402:UQ:H272	1.95	0.47
26:s:90:PRO:HD2	26:s:240:ILE:HD13	1.97	0.47
11:c:96:ASP:OD1	11:c:96:ASP:N	2.47	0.47
17:i:14:MET:O	17:i:18:MET:HG2	2.15	0.47
17:i:307:SER:OG	17:i:308:THR:N	2.48	0.47
27:u:83:THR:HA	27:u:86:TRP:NE1	2.30	0.47
20:l:435:PRO:HB3	20:l:437:PHE:CZ	2.50	0.47
25:r:76:MET:SD	25:r:230:VAL:HB	2.55	0.47
4:V:67:GLY:HA2	31:V:201:CDL:H221	1.97	0.46
20:l:295:GLN:HB2	20:l:301:ILE:HG12	1.96	0.46
9:a:163:ARG:NH2	15:g:95:TYR:OH	2.45	0.46
16:h:106:PRO:HG2	27:u:17:GLU:OE1	2.15	0.46
20:l:68:TRP:CD2	30:l:703:PEE:H42	2.49	0.46
31:o:201:CDL:H862	25:r:210:TYR:CE2	2.50	0.46
12:d:43:ARG:HB3	12:d:44:PRO:HD3	1.95	0.46
20:l:176:ARG:CG	25:r:401:MET:HA	2.44	0.46
20:l:311:GLY:O	20:l:315:VAL:HG13	2.16	0.46
33:r:502:PLX:H121	33:r:502:PLX:H92	1.70	0.46
30:j:201:PEE:H35	30:j:201:PEE:H30	1.65	0.46
25:r:271:MET:HE2	25:r:271:MET:HA	1.98	0.46
33:r:502:PLX:H101	33:r:502:PLX:H72	1.69	0.46
3:U:66:VAL:O	27:u:130:LYS:HE3	2.14	0.46
9:a:147:ALA:HB2	25:r:173:SER:HB2	1.97	0.46
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.97	0.46
20:l:407:TRP:O	20:l:411:MET:HG2	2.16	0.46
30:U:401:PEE:H59	26:s:277:TYR:CE2	2.51	0.46
9:a:96:ALA:HB2	12:d:61:TYR:CE2	2.51	0.46
33:j:203:PLX:H132	33:j:203:PLX:H161	1.60	0.46
31:k:101:CDL:H581	31:k:101:CDL:H611	1.70	0.46
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.45	0.46
13:e:74:HIS:HB2	13:e:83:ASP:OD2	2.16	0.46
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.97	0.46
9:a:139:ILE:HG23	25:r:54:LEU:HD23	1.96	0.46
31:a:201:CDL:H211	31:a:201:CDL:H182	1.60	0.46
15:g:85:TYR:CZ	27:u:165:SER:HB2	2.51	0.46
20:l:395:ILE:O	20:l:399:VAL:HG23	2.15	0.46
1:Q:53:TYR:OH	17:i:295:ARG:NH2	2.49	0.46
7:Y:78:ASP:OD1	7:Y:79:ALA:N	2.49	0.46
13:e:108:TYR:CE1	33:e:201:PLX:H1B1	2.51	0.46
17:i:40:MET:HE1	17:i:129:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:44:PHE:HB2	20:l:94:LEU:HB3	1.97	0.46
5:W:85:GLN:HG3	27:u:10:LEU:HD22	1.98	0.46
13:e:73:SER:O	13:e:75:GLY:N	2.49	0.46
20:l:166:THR:CG2	30:l:702:PEE:H2	2.45	0.46
22:n:11:HIS:HD2	22:n:14:HIS:HE1	1.63	0.46
26:s:102:VAL:HG21	26:s:154:LEU:HD11	1.98	0.46
27:u:59:GLU:OE1	27:u:59:GLU:N	2.44	0.46
11:c:126:TRP:O	11:c:127:ASN:HB2	2.16	0.45
9:a:60:SER:HB2	24:p:107:TRP:HA	1.98	0.45
14:f:68:GLU:HG2	15:g:21:ARG:HE	1.80	0.45
16:h:86:LEU:HB3	16:h:92:TYR:HB3	1.97	0.45
18:j:20:ILE:HG13	33:j:202:PLX:H142	1.98	0.45
25:r:116:ILE:HG13	27:u:168:PHE:CD2	2.52	0.45
13:e:108:TYR:CE1	33:e:201:PLX:C1B	3.00	0.45
33:j:202:PLX:H282	33:j:202:PLX:H251	1.91	0.45
29:w:45:LEU:O	29:w:45:LEU:HD12	2.17	0.45
9:a:184:LYS:C	9:a:186:THR:H	2.25	0.45
16:h:18:MET:HE1	19:k:59:MET:HB3	1.98	0.45
18:j:97:LEU:HD21	33:j:203:PLX:H391	1.98	0.45
2:S:12:MET:HE2	2:S:12:MET:HB3	1.74	0.45
19:k:28:SER:HB3	21:m:23:LYS:HG2	1.99	0.45
20:l:331:MET:HE2	20:l:331:MET:HA	1.97	0.45
23:o:116:ILE:CG1	23:o:121:LEU:HD22	2.47	0.45
20:l:312:LEU:O	20:l:315:VAL:HG22	2.16	0.45
25:r:201:MET:HE2	30:r:501:PEE:H78	0.59	0.45
15:g:77:LEU:HD11	33:g:201:PLX:H291	1.98	0.45
30:j:201:PEE:H58	30:j:201:PEE:H64	1.55	0.45
31:l:701:CDL:H712	31:l:701:CDL:H742	1.53	0.45
21:m:34:ILE:HG13	21:m:64:MET:HG3	1.97	0.45
23:o:23:TYR:OH	24:p:68:GLU:HG3	2.16	0.45
33:r:502:PLX:H6	33:r:502:PLX:H51	1.42	0.45
33:g:201:PLX:H71	33:g:201:PLX:H102	1.53	0.45
18:j:106:TRP:CE3	30:j:201:PEE:H20	2.52	0.45
30:j:201:PEE:O4	30:j:201:PEE:H3	2.16	0.45
25:r:235:LEU:O	25:r:238:LEU:HB2	2.17	0.45
6:X:71:ALA:HB2	20:l:442:LEU:HD11	1.99	0.45
18:j:73:LEU:N	18:j:74:PRO:HD2	2.32	0.44
18:j:105:GLU:HG3	18:j:110:GLY:HA3	1.99	0.44
13:e:108:TYR:CD1	33:e:201:PLX:H1B1	2.51	0.44
17:i:268:GLN:O	17:i:271:THR:OG1	2.33	0.44
20:l:468:ILE:O	20:l:472:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:186:PHE:O	26:s:189:THR:OG1	2.34	0.44
2:S:31:ASN:ND2	2:S:36:LYS:HB2	2.33	0.44
9:a:170:GLN:O	15:g:6:GLY:HA3	2.18	0.44
15:g:101:GLU:H	15:g:101:GLU:CD	2.25	0.44
17:i:255:PRO:HG3	17:i:260:PHE:CD1	2.52	0.44
20:l:384:PRO:HA	20:l:389:PHE:CD1	2.52	0.44
33:r:502:PLX:H1C3	33:r:502:PLX:H22	1.72	0.44
9:a:66:ARG:NH1	13:e:72:ASP:HB2	2.31	0.44
12:d:111:LYS:HD3	20:l:197:ASP:OD2	2.18	0.44
20:l:53:MET:HE2	20:l:59:GLN:HE22	1.83	0.44
23:o:84:PRO:HG3	31:o:201:CDL:H522	1.99	0.44
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.53	0.44
25:r:210:TYR:CG	25:r:268:GLY:HA3	2.53	0.44
31:r:503:CDL:H812	31:r:503:CDL:H841	1.90	0.44
29:w:139:ARG:NH1	29:w:166:ASP:OD1	2.46	0.44
3:U:59:ASP:CG	27:u:130:LYS:HD3	2.42	0.44
10:b:123:PHE:CZ	28:v:61:HIS:HB2	2.53	0.44
13:e:76:TYR:OH	36:e:301:HOH:O	2.15	0.44
17:i:59:TYR:O	17:i:63:GLN:HG2	2.17	0.44
17:i:68:MET:HE2	17:i:68:MET:HA	1.98	0.44
25:r:346:ARG:O	25:r:419:TYR:HA	2.18	0.44
27:u:38:LYS:HB3	27:u:39:PRO:HD3	1.99	0.44
28:v:17:PRO:HG2	28:v:102:PHE:CZ	2.53	0.44
16:h:21:GLN:HG3	19:k:53:PHE:HD1	1.83	0.44
25:r:185:PRO:HB3	25:r:252:PRO:HD3	2.00	0.44
29:w:66:ILE:O	29:w:214:ILE:HD12	2.17	0.44
30:Q:101:PEE:H60	30:Q:101:PEE:C23	2.39	0.44
7:Y:43:ARG:HH11	7:Y:49:GLN:HB2	1.82	0.44
20:l:358:LYS:HG3	24:p:80:TYR:CE1	2.52	0.44
31:l:701:CDL:H602	31:l:701:CDL:H571	1.85	0.44
31:o:201:CDL:H571	31:o:201:CDL:H732	1.99	0.44
25:r:445:LEU:HB3	31:r:503:CDL:H452	2.00	0.44
29:w:65:ASN:OD1	29:w:66:ILE:N	2.42	0.44
12:d:111:LYS:NZ	20:l:200:GLN:OE1	2.44	0.44
16:h:21:GLN:HA	19:k:53:PHE:CD1	2.53	0.44
17:i:62:THR:HG21	17:i:114:TRP:CD1	2.53	0.44
17:i:67:SER:OG	36:i:402:HOH:O	2.20	0.44
17:i:72:MET:HE3	17:i:76:ILE:HD11	1.99	0.44
23:o:83:THR:HG22	23:o:85:LYS:H	1.83	0.44
14:f:47:THR:HG23	15:g:65:LEU:HD22	1.99	0.44
5:W:55:ARG:NH2	26:s:311:THR:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:190:MET:CE	17:i:205:LEU:HA	2.48	0.43
20:l:67:HIS:NE2	20:l:70:THR:OG1	2.50	0.43
26:s:81:LEU:O	26:s:85:MET:HG2	2.19	0.43
7:Y:100:LEU:HB2	28:v:111:ARG:NH1	2.33	0.43
9:a:68:LEU:HD13	31:r:503:CDL:HB32	2.00	0.43
11:c:82:SER:HA	11:c:112:TYR:HB3	2.00	0.43
25:r:76:MET:HE1	36:r:651:HOH:O	2.18	0.43
22:n:4:VAL:HG22	22:n:8:VAL:HG23	1.99	0.43
26:s:236:ALA:HB1	26:s:259:PHE:CZ	2.53	0.43
8:Z:18:ASP:O	8:Z:21:GLN:HG2	2.18	0.43
9:a:135:LYS:NZ	22:n:32:ASP:OD1	2.35	0.43
31:l:701:CDL:H612	31:l:701:CDL:H641	1.80	0.43
13:e:73:SER:C	13:e:75:GLY:H	2.26	0.43
29:w:54:THR:C	29:w:56:THR:H	2.26	0.43
29:w:132:GLN:NE2	29:w:166:ASP:OD2	2.51	0.43
29:w:165:SER:O	29:w:168:VAL:HG22	2.18	0.43
2:S:34:LYS:NZ	2:S:61:HIS:HB2	2.34	0.43
7:Y:44:TYR:O	7:Y:45:ARG:HB2	2.19	0.43
8:Z:32:VAL:HG13	24:p:39:TYR:HB2	2.00	0.43
12:d:51:PHE:O	12:d:55:GLN:HG2	2.19	0.43
13:e:97:ILE:O	13:e:101:LEU:HB2	2.18	0.43
16:h:95:PRO:HG2	16:h:98:HIS:HD2	1.84	0.43
17:i:95:MET:HE1	17:i:145:ILE:HD12	2.01	0.43
26:s:180:PRO:O	26:s:183:MET:HB2	2.18	0.43
34:s:402:UQ:H262	34:s:402:UQ:H221	1.54	0.43
29:w:40:PRO:O	29:w:44:VAL:HG23	2.18	0.43
31:a:201:CDL:OB3	33:e:201:PLX:H1B2	2.18	0.43
33:e:201:PLX:H352	25:r:443:PRO:HB3	2.01	0.43
16:h:38:LYS:HE2	16:h:42:GLU:OE2	2.19	0.43
17:i:278:MET:HE3	17:i:278:MET:HB3	1.95	0.43
18:j:110:GLY:HA3	21:m:169:MET:HE1	2.00	0.43
21:m:2:THR:C	21:m:4:TYR:H	2.27	0.43
24:p:119:PHE:O	24:p:123:GLU:HG2	2.19	0.43
30:W:201:PEE:H42	30:W:201:PEE:H33	2.01	0.43
18:j:70:ALA:HA	21:m:55:MET:CE	2.49	0.43
20:l:63:ILE:O	20:l:79:SER:HA	2.18	0.43
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.54	0.43
20:l:331:MET:HG3	20:l:391:SER:HB2	1.99	0.43
26:s:233:MET:HE1	26:s:234:MET:HE2	2.01	0.43
29:w:110:GLY:HA2	29:w:134:TRP:CE2	2.54	0.43
29:w:176:GLN:NE2	29:w:236:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:V:201:CDL:H552	17:i:164:ILE:HD11	2.01	0.43
5:W:128:ARG:HB3	5:W:132:GLU:OE2	2.19	0.43
8:Z:63:PHE:CZ	20:l:424:THR:HG23	2.54	0.43
13:e:70:ASN:O	13:e:73:SER:HB3	2.19	0.43
20:l:327:LEU:O	20:l:331:MET:HG2	2.19	0.43
20:l:568:PHE:O	20:l:572:LYS:HG2	2.19	0.43
3:U:33:PRO:HA	26:s:310:MET:HG2	2.01	0.43
4:V:38:ALA:HA	31:k:101:CDL:H201	2.00	0.43
5:W:85:GLN:O	5:W:89:GLU:HG3	2.19	0.43
20:l:298:ILE:O	20:l:302:VAL:HG23	2.19	0.43
27:u:34:ALA:HB2	27:u:120:PRO:HG3	2.01	0.43
20:l:12:LEU:HD22	20:l:129:MET:HB3	1.99	0.42
20:l:230:HIS:N	20:l:231:PRO:HD3	2.33	0.42
11:c:169:GLU:OE2	28:v:43:GLN:HG3	2.19	0.42
15:g:13:LEU:HD23	33:g:201:PLX:H31	2.01	0.42
15:g:85:TYR:CZ	17:i:344:SER:HB3	2.53	0.42
16:h:80:LYS:NZ	21:m:1:MET:HE3	2.34	0.42
17:i:75:ILE:HD12	19:k:40:LEU:HD22	2.02	0.42
17:i:88:LYS:HD2	17:i:147:GLN:NE2	2.34	0.42
17:i:276:ILE:C	17:i:279:PRO:HD2	2.44	0.42
33:j:203:PLX:H1C3	33:j:203:PLX:H22	1.70	0.42
33:g:201:PLX:H351	17:i:339:MET:HB2	2.01	0.42
20:l:233:LEU:HB3	20:l:234:PRO:HD3	2.01	0.42
31:o:201:CDL:H111	31:o:201:CDL:H142	1.59	0.42
31:r:503:CDL:H581	31:r:503:CDL:H611	1.59	0.42
4:V:81:ARG:NH2	4:V:89:ASN:OD1	2.52	0.42
15:g:15:PHE:HB2	33:g:201:PLX:H6	2.01	0.42
29:w:170:LEU:HD22	29:w:187:TYR:CD1	2.54	0.42
13:e:63:ASP:N	13:e:63:ASP:OD1	2.52	0.42
33:g:201:PLX:H361	33:g:201:PLX:H311	2.01	0.42
17:i:1:MET:N	29:w:289:ARG:HH21	2.18	0.42
17:i:142:LEU:HB3	17:i:194:LEU:HD21	2.01	0.42
36:j:317:HOH:O	21:m:59:ILE:CD1	2.66	0.42
26:s:100:LEU:HD13	26:s:103:LEU:HD12	2.00	0.42
27:u:47:ARG:HD2	27:u:47:ARG:HA	1.87	0.42
28:v:27:PRO:O	28:v:34:ARG:NH1	2.52	0.42
11:c:153:TYR:OH	28:v:8:ARG:HD3	2.20	0.42
17:i:207:ILE:HD11	17:i:261:MET:CE	2.48	0.42
19:k:64:LEU:HD21	21:m:56:VAL:HG23	2.02	0.42
33:n:101:PLX:H22	33:n:101:PLX:H1C3	1.79	0.42
26:s:264:LEU:O	26:s:268:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:93:TYR:O	29:w:96:SER:OG	2.37	0.42
30:l:703:PEE:H39	30:l:703:PEE:H33	1.86	0.42
22:n:4:VAL:HA	22:n:7:ILE:HG12	2.02	0.42
29:w:83:LEU:HD22	29:w:156:GLY:HA3	2.02	0.42
1:Q:58:THR:HG23	1:Q:61:TRP:CD2	2.55	0.42
25:r:119:TYR:CZ	25:r:161:LEU:HB2	2.55	0.42
25:r:455:LEU:HA	25:r:455:LEU:HD23	1.85	0.42
31:r:504:CDL:H542	31:r:504:CDL:H511	1.75	0.42
31:s:401:CDL:H771	31:s:401:CDL:H801	1.81	0.42
27:u:152:PRO:O	27:u:153:GLU:HB2	2.17	0.42
9:a:168:TRP:CD2	15:g:3:MET:HE3	2.55	0.42
17:i:18:MET:HA	17:i:18:MET:HE3	2.02	0.42
17:i:320:THR:OG1	29:w:300:ASN:HA	2.20	0.42
31:k:101:CDL:H131	31:k:101:CDL:H161	1.80	0.42
20:l:383:MET:SD	20:l:384:PRO:HD2	2.59	0.42
23:o:107:THR:HG22	23:o:111:LYS:HE3	2.02	0.42
26:s:209:SER:HB3	26:s:213:VAL:HA	2.02	0.42
26:s:307:LEU:HA	26:s:310:MET:HE3	2.02	0.42
20:l:389:PHE:O	20:l:393:ASP:HB3	2.20	0.42
24:p:97:TYR:HB2	24:p:178:PRO:HG2	2.01	0.42
29:w:43:PHE:O	29:w:48:ARG:NH2	2.53	0.42
1:Q:47:PHE:CD1	1:Q:52:MET:HE1	2.53	0.41
7:Y:78:ASP:O	7:Y:82:GLY:N	2.47	0.41
13:e:65:ASN:HD21	13:e:67:TYR:HB2	1.85	0.41
20:l:560:THR:O	20:l:565:THR:OG1	2.34	0.41
27:u:80:GLU:HB2	27:u:81:PRO:HD3	2.02	0.41
31:V:201:CDL:H542	31:V:201:CDL:H511	1.89	0.41
9:a:136:THR:OG1	25:r:51:ASN:ND2	2.47	0.41
31:a:201:CDL:H342	31:a:201:CDL:H372	1.77	0.41
13:e:76:TYR:HB2	13:e:83:ASP:OD1	2.20	0.41
31:k:101:CDL:H131	20:l:589:LEU:HD21	2.02	0.41
20:l:174:TYR:CD2	20:l:232:TRP:HB3	2.56	0.41
30:Q:101:PEE:H28	30:Q:101:PEE:H36	2.02	0.41
30:W:201:PEE:H46	30:W:201:PEE:H39	1.92	0.41
10:b:121:LYS:HD3	28:v:40:VAL:HA	2.02	0.41
17:i:85:THR:HG22	17:i:87:THR:HG23	2.02	0.41
17:i:95:MET:HE2	17:i:149:ILE:HG22	2.02	0.41
20:l:49:VAL:HB	20:l:50:PRO:HD3	2.01	0.41
24:p:140:LEU:HD23	24:p:140:LEU:HA	1.88	0.41
25:r:266:MET:HB3	25:r:395:LEU:HD13	2.02	0.41
29:w:354:LEU:HD23	29:w:354:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:36:GLN:HA	25:r:138:ASN:ND2	2.35	0.41
13:e:55:LEU:HD21	29:w:320:GLY:HA3	2.03	0.41
13:e:57:GLU:HG3	13:e:58:ASP:O	2.19	0.41
17:i:261:MET:HB2	17:i:337:LEU:HD12	2.02	0.41
20:l:529:TYR:HB3	20:l:530:PRO:HD3	2.02	0.41
9:a:87:THR:HG23	31:a:201:CDL:HA61	2.02	0.41
11:c:85:GLU:OE1	11:c:119:THR:OG1	2.32	0.41
19:k:23:ARG:HG3	21:m:23:LYS:HE2	2.02	0.41
24:p:62:GLN:O	24:p:66:GLN:OE1	2.38	0.41
29:w:56:THR:HG22	29:w:83:LEU:HD21	2.03	0.41
6:X:136:GLU:OE2	24:p:18:ARG:NH2	2.53	0.41
9:a:152:LYS:HD3	15:g:96:VAL:HG21	2.01	0.41
16:h:7:GLN:O	16:h:11:GLY:N	2.53	0.41
20:l:152:PHE:CD1	20:l:168:ALA:HB1	2.56	0.41
26:s:3:MET:HE3	26:s:3:MET:HB3	1.90	0.41
26:s:17:VAL:HG13	26:s:228:TYR:HB2	2.01	0.41
10:b:87:LYS:HD3	10:b:88:TYR:CZ	2.56	0.41
33:j:202:PLX:H371	33:j:202:PLX:H342	1.86	0.41
23:o:53:ASP:HB3	23:o:56:ARG:HB2	2.02	0.41
26:s:221:ALA:O	26:s:225:MET:HG3	2.21	0.41
31:s:401:CDL:H182	31:s:401:CDL:H362	2.02	0.41
10:b:88:TYR:CE1	12:d:49:ARG:HG2	2.56	0.41
12:d:37:PHE:CD1	20:l:3:PRO:HB3	2.56	0.41
20:l:557:TRP:O	20:l:561:ILE:HG12	2.20	0.41
25:r:3:LYS:HB3	25:r:3:LYS:HE3	1.84	0.41
5:W:94:GLU:OE1	5:W:106:VAL:HG13	2.21	0.41
9:a:94:GLY:O	12:d:61:TYR:OH	2.38	0.41
11:c:127:ASN:O	11:c:131:LYS:HE2	2.20	0.41
18:j:5:LEU:HD21	26:s:3:MET:SD	2.61	0.41
20:l:332:HIS:HA	20:l:335:PHE:CZ	2.56	0.41
22:n:54:GLU:HG2	22:n:55:VAL:N	2.35	0.41
25:r:52:PHE:CE2	25:r:58:SER:HB2	2.56	0.41
26:s:24:GLU:O	26:s:28:LEU:HG	2.20	0.41
28:v:14:SER:O	28:v:109:LEU:HD21	2.21	0.41
30:W:201:PEE:H38	30:W:201:PEE:H32	1.60	0.41
11:c:78:LEU:HB2	11:c:106:HIS:CD2	2.56	0.41
13:e:86:ASN:C	13:e:86:ASN:HD22	2.27	0.41
17:i:287:LEU:HD23	17:i:287:LEU:HA	1.86	0.41
17:i:321:LYS:HE2	17:i:321:LYS:HB2	1.90	0.41
20:l:79:SER:OG	20:l:135:ASN:HB3	2.21	0.41
26:s:100:LEU:HB3	26:s:103:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:71:PRO:HA	1:Q:72:PRO:HD3	1.96	0.40
6:X:89:LEU:HD13	8:Z:48:ASN:HA	2.02	0.40
9:a:106:VAL:CG1	22:n:50:ARG:HE	2.34	0.40
15:g:48:ASN:HB3	15:g:55:VAL:HA	2.04	0.40
18:j:12:THR:O	18:j:16:LEU:HD23	2.21	0.40
26:s:81:LEU:HD11	26:s:111:LEU:HG	2.03	0.40
13:e:53:ILE:HG22	13:e:55:LEU:H	1.86	0.40
25:r:63:ALA:HA	25:r:66:LEU:HD12	2.03	0.40
7:Y:61:PHE:CZ	20:l:455:LYS:HG3	2.56	0.40
9:a:171:TYR:OH	15:g:1:MET:N	2.54	0.40
11:c:38:PRO:HD3	23:o:67:ARG:HG2	2.03	0.40
12:d:142:ARG:NE	13:e:138:GLU:O	2.50	0.40
17:i:243:LEU:HD22	17:i:330:ILE:HG21	2.02	0.40
20:l:229:LEU:HD21	30:l:702:PEE:H36	2.04	0.40
25:r:138:ASN:HD22	25:r:138:ASN:C	2.28	0.40
25:r:438:ALA:HA	25:r:441:ILE:HG22	2.02	0.40
31:r:503:CDL:H511	31:r:503:CDL:HA31	2.02	0.40
29:w:221:LYS:CA	29:w:221:LYS:CE	2.85	0.40
6:X:129:GLU:HB3	24:p:82:PHE:CD2	2.57	0.40
24:p:59:LYS:O	24:p:62:GLN:HG3	2.22	0.40
25:r:71:TRP:O	25:r:74:PRO:HD2	2.21	0.40
31:r:503:CDL:H192	31:r:503:CDL:H161	1.81	0.40
7:Y:61:PHE:HE2	20:l:455:LYS:HE2	1.86	0.40
13:e:55:LEU:CD2	13:e:57:GLU:HB2	2.52	0.40
17:i:244:MET:HE3	17:i:244:MET:HB2	1.98	0.40
30:l:703:PEE:H34	31:r:503:CDL:H242	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
3	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
4	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
5	W	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
6	X	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
7	Y	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	Z	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
9	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
10	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
11	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
12	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
13	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
14	f	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
15	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
16	h	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
17	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
18	j	113/115 (98%)	107 (95%)	5 (4%)	1 (1%)	14	30
19	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
20	l	604/606 (100%)	589 (98%)	14 (2%)	1 (0%)	43	66
21	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
24	p	176/178 (99%)	172 (98%)	3 (2%)	1 (1%)	21	42
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	316/318 (99%)	302 (96%)	13 (4%)	1 (0%)	36	58
27	u	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	21	42
28	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
29	w	318/320 (99%)	310 (98%)	8 (2%)	0	100	100
All	All	4667/4756 (98%)	4506 (97%)	156 (3%)	5 (0%)	49	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	l	72	GLN
26	s	208	VAL
18	j	40	GLY
24	p	174	PRO
27	u	152	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	38/38 (100%)	38 (100%)	0	100	100
2	S	57/58 (98%)	57 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	101/101 (100%)	101 (100%)	0	100	100
5	W	99/99 (100%)	99 (100%)	0	100	100
6	X	78/81 (96%)	78 (100%)	0	100	100
7	Y	62/62 (100%)	62 (100%)	0	100	100
8	Z	62/62 (100%)	62 (100%)	0	100	100
9	a	121/121 (100%)	121 (100%)	0	100	100
10	b	90/119 (76%)	90 (100%)	0	100	100
11	c	141/141 (100%)	141 (100%)	0	100	100
12	d	155/155 (100%)	155 (100%)	0	100	100
13	e	96/96 (100%)	96 (100%)	0	100	100
14	f	36/45 (80%)	36 (100%)	0	100	100
15	g	108/109 (99%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	311 (100%)	0	100	100
18	j	100/100 (100%)	100 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	538/540 (100%)	538 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	m	131/141 (93%)	131 (100%)	0	100	100
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	159/159 (100%)	159 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	275/275 (100%)	273 (99%)	2 (1%)	76	89
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	108/111 (97%)	108 (100%)	0	100	100
29	w	283/283 (100%)	283 (100%)	0	100	100
All	All	4125/4183 (99%)	4123 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	s	202	GLU
26	s	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
5	W	76	GLN
8	Z	21	GLN
11	c	84	GLN
11	c	183	HIS
12	d	131	GLN
13	e	86	ASN
13	e	115	GLN
13	e	145	ASN
14	f	61	GLN
16	h	98	HIS
17	i	147	GLN
17	i	171	ASN
17	i	232	HIS
17	i	268	GLN
17	i	289	ASN
19	k	50	ASN
20	l	135	ASN
20	l	199	GLN

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Mol	Chain	Res	Type
20	l	348	HIS
20	l	354	GLN
20	l	541	ASN
20	l	580	GLN
20	l	603	ASN
22	n	11	HIS
23	o	52	ASN
24	p	78	GLN
25	r	30	HIS
25	r	81	GLN
25	r	138	ASN
25	r	399	ASN
26	s	5	ASN
26	s	47	GLN
26	s	99	ASN
26	s	194	ASN
26	s	250	HIS
27	u	65	GLN
29	w	132	GLN
29	w	219	GLN
29	w	300	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PEE	U	401	-	50,50,50	1.17	6 (12%)	53,55,55	1.01	2 (3%)
30	PEE	Q	101	-	46,46,50	1.23	6 (13%)	49,51,55	1.01	3 (6%)
30	PEE	l	703	-	45,45,50	1.25	6 (13%)	48,50,55	1.00	2 (4%)
30	PEE	l	702	-	49,49,50	1.18	6 (12%)	52,54,55	0.96	2 (3%)
31	CDL	o	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	5 (4%)
34	UQ	s	402	-	38,38,63	3.63	9 (23%)	48,49,79	2.79	17 (35%)
31	CDL	r	503	-	98,98,99	1.11	8 (8%)	104,110,111	0.89	4 (3%)
31	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.91	4 (3%)
31	CDL	r	504	-	75,75,99	1.22	8 (10%)	81,87,111	0.97	4 (4%)
31	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.85	4 (4%)
31	CDL	k	101	-	99,99,99	1.11	8 (8%)	105,111,111	0.82	4 (3%)
33	PLX	j	203	-	51,51,51	1.20	5 (9%)	53,59,59	0.61	1 (1%)
33	PLX	n	101	-	51,51,51	1.23	4 (7%)	53,59,59	0.60	1 (1%)
31	CDL	l	701	-	87,87,99	1.16	8 (9%)	93,99,111	0.90	4 (4%)
32	8Q1	X	201	-	32,34,34	2.24	7 (21%)	39,43,43	1.76	13 (33%)
33	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.63	2 (3%)
31	CDL	u	201	-	54,54,99	1.23	4 (7%)	60,66,111	1.26	5 (8%)
33	PLX	e	201	-	51,51,51	0.62	0	53,59,59	0.63	0
30	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.93	2 (3%)
33	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.63	1 (1%)
30	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
30	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
35	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.87	8 (18%)
31	CDL	s	401	-	88,88,99	1.15	8 (9%)	94,100,111	0.93	4 (4%)
33	PLX	g	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.64	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PEE	U	401	-	-	25/54/54/54	-
30	PEE	Q	101	-	-	26/50/50/54	-
30	PEE	l	703	-	-	21/49/49/54	-
30	PEE	l	702	-	-	22/53/53/54	-
31	CDL	o	201	-	-	55/110/110/110	-
34	UQ	s	402	-	-	13/33/57/87	0/1/1/1
31	CDL	r	503	-	-	58/109/109/110	-
31	CDL	a	201	-	-	65/110/110/110	-
31	CDL	r	504	-	-	43/86/86/110	-
31	CDL	V	201	-	-	57/104/104/110	-
31	CDL	k	101	-	-	56/110/110/110	-
33	PLX	j	203	-	-	27/55/55/55	-
33	PLX	n	101	-	-	30/55/55/55	-
31	CDL	l	701	-	-	42/98/98/110	-
32	8Q1	X	201	-	-	10/41/41/41	-
33	PLX	j	202	-	-	27/55/55/55	-
31	CDL	u	201	-	-	17/65/65/110	-
33	PLX	e	201	-	-	18/55/55/55	-
30	PEE	j	201	-	-	23/54/54/54	-
33	PLX	r	502	-	-	24/55/55/55	-
30	PEE	W	201	-	-	23/44/44/54	-
30	PEE	r	501	-	-	29/54/54/54	-
35	ADP	w	401	-	-	5/16/32/32	0/3/3/3
31	CDL	s	401	-	-	43/99/99/110	-
33	PLX	g	201	-	-	27/55/55/55	-

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C18-C19	10.00	1.56	1.33
34	s	402	UQ	C13-C14	9.64	1.55	1.33
34	s	402	UQ	C23-C24	9.41	1.54	1.33
34	s	402	UQ	C8-C9	9.29	1.54	1.33
35	w	401	ADP	C3'-C4'	-9.08	1.30	1.53
35	w	401	ADP	O4'-C4'	7.82	1.62	1.45
32	X	201	8Q1	P24-O27	7.53	1.84	1.60
34	s	402	UQ	C28-C29	7.34	1.54	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	w	401	ADP	PA-O3A	6.57	1.66	1.59
35	w	401	ADP	C6-N6	5.44	1.48	1.34
32	X	201	8Q1	C28-C29	5.14	1.61	1.52
35	w	401	ADP	O4'-C1'	-4.38	1.31	1.42
31	u	201	CDL	OA8-CA7	4.19	1.45	1.33
31	u	201	CDL	OB8-CB7	4.14	1.45	1.33
31	u	201	CDL	OA6-CA5	4.12	1.45	1.34
31	u	201	CDL	OB6-CB5	4.09	1.45	1.34
32	X	201	8Q1	C1-S44	3.85	1.85	1.76
30	Q	101	PEE	C18-C19	3.83	1.53	1.31
30	r	501	PEE	C18-C19	3.82	1.53	1.31
30	l	703	PEE	C18-C19	3.82	1.53	1.31
30	j	201	PEE	C18-C19	3.81	1.53	1.31
30	l	702	PEE	C18-C19	3.81	1.53	1.31
30	U	401	PEE	C18-C19	3.79	1.53	1.31
30	W	201	PEE	C18-C19	3.78	1.53	1.31
30	r	501	PEE	C39-C38	3.74	1.52	1.31
30	Q	101	PEE	C39-C38	3.74	1.52	1.31
30	U	401	PEE	C39-C38	3.72	1.52	1.31
30	j	201	PEE	C39-C38	3.72	1.52	1.31
30	l	703	PEE	C39-C38	3.70	1.52	1.31
30	l	702	PEE	C39-C38	3.68	1.52	1.31
31	r	503	CDL	OA8-CA7	3.53	1.43	1.33
31	l	701	CDL	OA8-CA7	3.47	1.43	1.33
31	V	201	CDL	OA8-CA7	3.46	1.43	1.33
31	a	201	CDL	OA8-CA7	3.45	1.43	1.33
32	X	201	8Q1	O27-C28	-3.43	1.32	1.43
31	o	201	CDL	OA8-CA7	3.42	1.43	1.33
32	X	201	8Q1	C34-N36	3.42	1.41	1.33
31	s	401	CDL	OA8-CA7	3.40	1.43	1.33
31	k	101	CDL	OA8-CA7	3.37	1.43	1.33
31	r	504	CDL	OA8-CA7	3.34	1.43	1.33
35	w	401	ADP	C8-N9	-3.31	1.31	1.37
31	k	101	CDL	OA6-CA5	3.20	1.43	1.34
35	w	401	ADP	O2'-C2'	-3.11	1.35	1.43
32	X	201	8Q1	C6-C1	3.09	1.54	1.50
31	V	201	CDL	OA6-CA5	3.07	1.42	1.34
32	X	201	8Q1	C39-N41	3.04	1.40	1.33
31	s	401	CDL	OA6-CA5	3.04	1.42	1.34
31	V	201	CDL	OB6-CB5	3.03	1.42	1.34
31	r	504	CDL	OB8-CB7	3.03	1.42	1.33
31	a	201	CDL	OB8-CB7	3.02	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	503	CDL	OB8-CB7	3.02	1.42	1.33
31	s	401	CDL	OB6-CB5	3.02	1.42	1.34
35	w	401	ADP	O3'-C3'	2.99	1.50	1.43
31	o	201	CDL	OA6-CA5	2.98	1.42	1.34
31	r	504	CDL	OB6-CB5	2.98	1.42	1.34
31	k	101	CDL	OB8-CB7	2.97	1.42	1.33
31	k	101	CDL	OB6-CB5	2.97	1.42	1.34
31	V	201	CDL	OB8-CB7	2.96	1.42	1.33
31	r	503	CDL	OB6-CB5	2.96	1.42	1.34
31	a	201	CDL	OB6-CB5	2.96	1.42	1.34
33	n	101	PLX	O6-C4	-2.95	1.40	1.44
31	l	701	CDL	OA6-CA5	2.93	1.42	1.34
31	r	504	CDL	OA6-CA5	2.92	1.42	1.34
31	a	201	CDL	OA6-CA5	2.92	1.42	1.34
31	l	701	CDL	OB6-CB5	2.90	1.42	1.34
31	o	201	CDL	OB6-CB5	2.88	1.42	1.34
31	s	401	CDL	OB8-CB7	2.88	1.41	1.33
31	o	201	CDL	OB8-CB7	2.88	1.41	1.33
31	l	701	CDL	OB8-CB7	2.87	1.41	1.33
31	r	503	CDL	OA6-CA5	2.85	1.42	1.34
33	g	201	PLX	O6-C4	-2.77	1.41	1.44
34	s	402	UQ	C6-C1	2.73	1.54	1.46
31	a	201	CDL	OA6-CA4	-2.72	1.40	1.46
31	r	504	CDL	OA6-CA4	-2.62	1.40	1.46
33	r	502	PLX	O6-C4	-2.62	1.41	1.44
30	W	201	PEE	O2-C2	-2.62	1.40	1.46
30	Q	101	PEE	O2-C2	-2.61	1.40	1.46
31	r	503	CDL	OA6-CA4	-2.60	1.40	1.46
31	s	401	CDL	OA6-CA4	-2.59	1.40	1.46
30	l	703	PEE	O2-C2	-2.59	1.40	1.46
31	o	201	CDL	OA6-CA4	-2.59	1.40	1.46
31	l	701	CDL	OA6-CA4	-2.58	1.40	1.46
33	j	203	PLX	O6-C4	-2.58	1.41	1.44
30	l	702	PEE	O2-C2	-2.57	1.40	1.46
30	j	201	PEE	O3-C30	2.55	1.40	1.33
30	U	401	PEE	O2-C2	-2.54	1.40	1.46
30	l	703	PEE	O3-C30	2.51	1.40	1.33
31	l	701	CDL	OB6-CB4	-2.49	1.40	1.46
30	r	501	PEE	O2-C2	-2.49	1.40	1.46
33	j	202	PLX	C7-C6	2.48	1.55	1.50
30	l	702	PEE	O3-C30	2.48	1.40	1.33
33	j	203	PLX	C7-C6	2.48	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	j	201	PEE	O2-C2	-2.47	1.40	1.46
31	r	503	CDL	OB6-CB4	-2.47	1.40	1.46
31	o	201	CDL	OB6-CB4	-2.46	1.40	1.46
33	n	101	PLX	C7-C6	2.45	1.55	1.50
31	k	101	CDL	OB6-CB4	-2.43	1.40	1.46
33	j	202	PLX	O6-C4	-2.41	1.41	1.44
33	g	201	PLX	C7-C6	2.41	1.55	1.50
30	Q	101	PEE	O3-C30	2.40	1.40	1.33
30	r	501	PEE	O3-C30	2.37	1.40	1.33
31	a	201	CDL	OB6-CB4	-2.36	1.41	1.46
33	r	502	PLX	C7-C6	2.34	1.55	1.50
30	W	201	PEE	O3-C3	-2.34	1.39	1.45
35	w	401	ADP	C5-N7	-2.34	1.34	1.39
30	W	201	PEE	O3-C30	2.33	1.40	1.33
30	Q	101	PEE	O2-C10	2.32	1.40	1.34
34	s	402	UQ	C7-C8	2.32	1.54	1.50
31	V	201	CDL	OA6-CA4	-2.32	1.41	1.46
31	r	504	CDL	OB6-CB4	-2.31	1.41	1.46
30	j	201	PEE	O2-C10	2.31	1.40	1.34
31	r	504	CDL	PB2-OB2	2.31	1.68	1.59
30	l	703	PEE	O2-C10	2.30	1.40	1.34
31	o	201	CDL	PB2-OB2	2.29	1.68	1.59
31	V	201	CDL	OB6-CB4	-2.29	1.41	1.46
31	V	201	CDL	PB2-OB5	2.28	1.68	1.59
31	s	401	CDL	OB6-CB4	-2.28	1.41	1.46
30	U	401	PEE	O3-C30	2.28	1.40	1.33
31	V	201	CDL	PB2-OB2	2.27	1.68	1.59
31	s	401	CDL	PB2-OB2	2.26	1.68	1.59
31	k	101	CDL	OA6-CA4	-2.26	1.41	1.46
31	r	503	CDL	PB2-OB2	2.22	1.68	1.59
30	r	501	PEE	O2-C10	2.22	1.40	1.34
31	o	201	CDL	PB2-OB5	2.22	1.68	1.59
30	r	501	PEE	O3-C3	-2.22	1.40	1.45
31	l	701	CDL	PB2-OB2	2.21	1.68	1.59
30	W	201	PEE	O2-C10	2.20	1.40	1.34
33	j	203	PLX	P1-O4	2.19	1.68	1.59
31	a	201	CDL	PB2-OB5	2.19	1.67	1.59
33	j	202	PLX	P1-O4	2.18	1.67	1.59
31	a	201	CDL	PB2-OB2	2.18	1.67	1.59
33	n	101	PLX	P1-O4	2.18	1.67	1.59
31	r	504	CDL	PB2-OB5	2.18	1.67	1.59
30	l	702	PEE	O3-C3	-2.17	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	U	401	PEE	O2-C10	2.16	1.40	1.34
33	r	502	PLX	P1-O1	2.15	1.67	1.59
33	g	201	PLX	P1-O4	2.15	1.67	1.59
31	k	101	CDL	PB2-OB5	2.15	1.67	1.59
31	r	503	CDL	PB2-OB5	2.15	1.67	1.59
30	l	702	PEE	O2-C10	2.14	1.40	1.34
31	k	101	CDL	PB2-OB2	2.13	1.67	1.59
33	r	502	PLX	P1-O4	2.12	1.67	1.59
34	s	402	UQ	O4-C4	-2.12	1.18	1.23
31	s	401	CDL	PB2-OB5	2.11	1.67	1.59
30	U	401	PEE	O3-C3	-2.11	1.40	1.45
31	l	701	CDL	PB2-OB5	2.10	1.67	1.59
33	j	203	PLX	P1-O1	2.09	1.67	1.59
30	Q	101	PEE	O3-C3	-2.09	1.40	1.45
33	n	101	PLX	P1-O1	2.08	1.67	1.59
34	s	402	UQ	O3-CM3	-2.06	1.40	1.45
33	r	502	PLX	C25-C24	2.05	1.55	1.50
31	V	201	CDL	C11-CA5	2.05	1.56	1.50
33	j	202	PLX	P1-O1	2.02	1.67	1.59
30	l	703	PEE	O3-C3	-2.02	1.40	1.45
33	j	203	PLX	C1-C2	2.01	1.57	1.51
30	j	201	PEE	O3-C3	-2.00	1.40	1.45
33	g	201	PLX	P1-O1	2.00	1.67	1.59

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	402	UQ	C7-C8-C9	-8.20	112.70	126.83
34	s	402	UQ	C17-C18-C19	-6.28	113.26	127.62
34	s	402	UQ	C12-C13-C14	-5.99	113.91	127.62
34	s	402	UQ	C22-C23-C24	-5.95	114.00	127.62
35	w	401	ADP	C5-C4-N3	-5.51	119.13	126.72
35	w	401	ADP	N3-C2-N1	-4.61	121.61	128.58
34	s	402	UQ	C27-C28-C29	-4.46	112.77	127.64
35	w	401	ADP	N3-C4-N9	4.33	134.54	127.17
34	s	402	UQ	C10-C9-C8	-4.26	112.68	123.63
30	U	401	PEE	O2-C10-C11	4.22	120.61	111.48
34	s	402	UQ	C25-C24-C23	-4.21	112.81	123.63
31	a	201	CDL	OB6-CB5-C51	4.19	120.54	111.48
34	s	402	UQ	C20-C19-C18	-4.17	112.92	123.63
32	X	201	8Q1	C6-C1-S44	4.17	118.37	113.40
30	l	703	PEE	O2-C10-C11	4.13	120.41	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	201	8Q1	C43-S44-C1	4.13	114.04	101.84
31	s	401	CDL	OB6-CB5-C51	4.05	120.25	111.48
31	u	201	CDL	OA6-CA5-C11	4.02	120.17	111.48
31	a	201	CDL	OA6-CA5-C11	4.01	120.15	111.48
31	r	504	CDL	OB6-CB5-C51	3.97	120.07	111.48
31	u	201	CDL	OB6-CB5-C51	3.97	120.07	111.48
31	V	201	CDL	OA6-CA5-C11	3.95	120.02	111.48
30	r	501	PEE	O2-C10-C11	3.94	120.00	111.48
31	o	201	CDL	OB6-CB5-C51	3.93	119.98	111.48
30	W	201	PEE	O2-C10-C11	3.93	119.98	111.48
30	Q	101	PEE	O2-C10-C11	3.92	119.97	111.48
31	s	401	CDL	OA6-CA5-C11	3.89	119.89	111.48
31	r	503	CDL	OA6-CA5-C11	3.85	119.82	111.48
31	r	503	CDL	OB6-CB5-C51	3.83	119.77	111.48
31	r	504	CDL	OA6-CA5-C11	3.82	119.74	111.48
31	o	201	CDL	OA6-CA5-C11	3.80	119.69	111.48
31	l	701	CDL	OB6-CB5-C51	3.80	119.69	111.48
31	V	201	CDL	OB6-CB5-C51	3.78	119.67	111.48
31	l	701	CDL	OA6-CA5-C11	3.75	119.59	111.48
34	s	402	UQ	C21-C19-C18	-3.74	112.76	121.17
30	j	201	PEE	O2-C10-C11	3.71	119.50	111.48
34	s	402	UQ	C15-C14-C13	-3.67	114.21	123.63
31	k	101	CDL	OB6-CB5-C51	3.66	119.41	111.48
35	w	401	ADP	C2-N3-C4	3.60	120.62	111.83
30	l	702	PEE	O2-C10-C11	3.60	119.26	111.48
34	s	402	UQ	C11-C9-C8	-3.53	113.25	121.17
34	s	402	UQ	C26-C24-C23	-3.48	113.36	121.17
34	s	402	UQ	C16-C14-C13	-3.47	113.38	121.17
35	w	401	ADP	N9-C8-N7	-3.43	109.06	113.94
31	k	101	CDL	OA6-CA5-C11	3.34	118.70	111.48
34	s	402	UQ	C30-C29-C28	-3.25	112.89	122.66
34	s	402	UQ	C31-C29-C28	-3.23	112.95	122.66
32	X	201	8Q1	O35-C34-N36	-3.22	116.17	122.98
31	u	201	CDL	OB8-CB7-C71	3.16	121.48	111.83
35	w	401	ADP	C5-N7-C8	3.16	108.41	103.45
35	w	401	ADP	C4-N9-C8	3.11	109.01	105.74
31	a	201	CDL	OB8-CB7-C71	2.99	120.96	111.83
30	l	702	PEE	O3-C30-C31	2.99	120.94	111.83
35	w	401	ADP	C4-C5-N7	-2.97	107.19	110.58
31	o	201	CDL	OB8-CB7-C71	2.91	120.70	111.83
31	r	503	CDL	OA8-CA7-C31	2.90	120.67	111.83
31	r	503	CDL	OB8-CB7-C71	2.87	120.59	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	504	CDL	OB8-CB7-C71	2.87	120.59	111.83
32	X	201	8Q1	O2-P24-O27	-2.87	99.20	106.67
31	k	101	CDL	OA8-CA7-C31	2.85	120.52	111.83
30	U	401	PEE	O3-C30-C31	2.84	120.48	111.83
31	k	101	CDL	OB8-CB7-C71	2.80	120.38	111.83
31	l	701	CDL	OB8-CB7-C71	2.80	120.37	111.83
30	j	201	PEE	O3-C30-C31	2.79	120.35	111.83
31	o	201	CDL	OA8-CA7-C31	2.73	120.16	111.83
30	Q	101	PEE	O3-C30-C31	2.72	120.14	111.83
31	r	504	CDL	OA8-CA7-C31	2.70	120.06	111.83
31	V	201	CDL	OB8-CB7-C71	2.67	119.97	111.83
31	s	401	CDL	OA8-CA7-C31	2.67	119.96	111.83
31	u	201	CDL	OA8-CA7-C31	2.66	119.23	111.15
30	r	501	PEE	O3-C30-C31	2.64	119.89	111.83
32	X	201	8Q1	C32-C34-N36	2.64	121.50	116.48
33	g	201	PLX	C1A-N1-C1	2.60	120.25	109.91
30	W	201	PEE	O3-C30-C31	2.59	119.72	111.83
31	l	701	CDL	OA8-CA7-C31	2.56	119.64	111.83
31	V	201	CDL	OA8-CA7-C31	2.55	119.61	111.83
32	X	201	8Q1	O40-C39-N41	-2.55	118.03	123.03
34	s	402	UQ	C7-C6-C5	-2.55	120.52	124.89
33	r	502	PLX	C1A-N1-C1	2.51	119.91	109.91
31	s	401	CDL	OB8-CB7-C71	2.50	119.45	111.83
30	l	703	PEE	O3-C30-C31	2.49	119.43	111.83
33	n	101	PLX	C1A-N1-C1	2.46	119.69	109.91
34	s	402	UQ	CM5-C5-C6	-2.43	120.45	124.45
32	X	201	8Q1	C37-C38-C39	2.43	116.44	112.39
31	a	201	CDL	OA8-CA7-C31	2.41	119.18	111.83
32	X	201	8Q1	C43-C42-N41	2.35	117.31	112.41
33	j	203	PLX	C1A-N1-C1	2.34	119.21	109.91
33	j	202	PLX	C1A-N1-C1	2.29	119.00	109.91
32	X	201	8Q1	O1-P24-O2	2.28	116.35	107.80
31	u	201	CDL	OB8-CB7-OB9	-2.26	117.97	123.63
32	X	201	8Q1	C38-C39-N41	2.24	120.43	116.34
32	X	201	8Q1	O27-P24-O3	-2.11	100.73	106.44
32	X	201	8Q1	O4-C1-S44	-2.08	120.04	122.68
32	X	201	8Q1	O4-C1-C6	-2.07	121.59	123.98
33	j	202	PLX	C2-C1-N1	-2.05	109.25	115.82
31	o	201	CDL	CB4-OB6-CB5	-2.00	113.00	117.80
30	Q	101	PEE	C2-O2-C10	-2.00	113.00	117.80

There are no chirality outliers.

All (786) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C11-C10-O2-C2
30	Q	101	PEE	C4-O4P-P-O2P
30	Q	101	PEE	C4-O4P-P-O1P
30	Q	101	PEE	C5-C4-O4P-P
30	U	401	PEE	C4-O4P-P-O3P
30	U	401	PEE	C4-O4P-P-O2P
30	W	201	PEE	C1-O3P-P-O2P
30	W	201	PEE	C1-O3P-P-O1P
30	W	201	PEE	C1-O3P-P-O4P
30	W	201	PEE	C4-O4P-P-O3P
30	W	201	PEE	C4-O4P-P-O2P
30	W	201	PEE	O4P-C4-C5-N
30	j	201	PEE	C4-O4P-P-O3P
30	j	201	PEE	C4-O4P-P-O1P
30	l	702	PEE	C11-C10-O2-C2
30	l	702	PEE	O4P-C4-C5-N
30	l	703	PEE	C1-O3P-P-O2P
30	l	703	PEE	C1-O3P-P-O1P
30	l	703	PEE	C1-O3P-P-O4P
30	l	703	PEE	O4P-C4-C5-N
30	r	501	PEE	C1-O3P-P-O2P
31	V	201	CDL	CA2-OA2-PA1-OA3
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	CA3-OA5-PA1-OA2
31	V	201	CDL	CA3-OA5-PA1-OA3
31	V	201	CDL	CA3-OA5-PA1-OA4
31	V	201	CDL	CB2-OB2-PB2-OB3
31	V	201	CDL	CB3-OB5-PB2-OB3
31	V	201	CDL	CB3-OB5-PB2-OB4
31	V	201	CDL	OB6-CB4-CB6-OB8
31	a	201	CDL	CA2-OA2-PA1-OA3
31	a	201	CDL	CA2-OA2-PA1-OA5
31	a	201	CDL	CA3-OA5-PA1-OA2
31	a	201	CDL	CA3-OA5-PA1-OA4
31	a	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CB3-OB5-PB2-OB2
31	a	201	CDL	CB3-OB5-PB2-OB3
31	a	201	CDL	CB3-OB5-PB2-OB4
31	k	101	CDL	CA3-OA5-PA1-OA2
31	k	101	CDL	CA3-OA5-PA1-OA3
31	k	101	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
31	k	101	CDL	OA5-CA3-CA4-OA6
31	k	101	CDL	CB2-OB2-PB2-OB3
31	k	101	CDL	CB2-OB2-PB2-OB5
31	l	701	CDL	CB2-OB2-PB2-OB3
31	l	701	CDL	CB2-OB2-PB2-OB4
31	l	701	CDL	CB2-OB2-PB2-OB5
31	o	201	CDL	CA2-OA2-PA1-OA5
31	o	201	CDL	CB3-OB5-PB2-OB2
31	o	201	CDL	CB3-OB5-PB2-OB3
31	o	201	CDL	CB3-OB5-PB2-OB4
31	o	201	CDL	OB5-CB3-CB4-OB6
31	r	503	CDL	CA2-C1-CB2-OB2
31	r	503	CDL	CA2-OA2-PA1-OA4
31	r	503	CDL	CA2-OA2-PA1-OA5
31	r	503	CDL	CA3-OA5-PA1-OA3
31	r	503	CDL	OA9-CA7-OA8-CA6
31	r	503	CDL	C31-CA7-OA8-CA6
31	r	503	CDL	CB2-OB2-PB2-OB3
31	r	503	CDL	CB2-OB2-PB2-OB4
31	r	503	CDL	CB3-OB5-PB2-OB3
31	r	504	CDL	CA3-OA5-PA1-OA2
31	r	504	CDL	CB2-OB2-PB2-OB4
31	r	504	CDL	CB3-OB5-PB2-OB2
31	r	504	CDL	CB3-OB5-PB2-OB3
31	r	504	CDL	CB3-OB5-PB2-OB4
31	r	504	CDL	C51-CB5-OB6-CB4
31	s	401	CDL	CA2-C1-CB2-OB2
31	s	401	CDL	OA5-CA3-CA4-OA6
31	s	401	CDL	C51-CB5-OB6-CB4
31	u	201	CDL	CA2-OA2-PA1-OA3
31	u	201	CDL	CA2-OA2-PA1-OA5
31	u	201	CDL	CA3-OA5-PA1-OA2
31	u	201	CDL	CB3-OB5-PB2-OB2
31	u	201	CDL	CB3-OB5-PB2-OB3
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	N41-C42-C43-S44
33	e	201	PLX	C3-O4-P1-O1
33	e	201	PLX	C3-O4-P1-O2
33	e	201	PLX	C2-O1-P1-O4
33	e	201	PLX	C2-O1-P1-O3
33	g	201	PLX	C3-O4-P1-O1
33	g	201	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C2-O1-P1-O4
33	g	201	PLX	C2-O1-P1-O2
33	g	201	PLX	C2-O1-P1-O3
33	j	202	PLX	O7-C6-O6-C4
33	j	202	PLX	C3-C4-O6-C6
33	j	202	PLX	N1-C1-C2-O1
33	j	202	PLX	C25-C24-O8-C5
33	j	203	PLX	O7-C6-C7-C8
33	j	203	PLX	C7-C6-O6-C4
33	j	203	PLX	C3-O4-P1-O1
33	j	203	PLX	C3-O4-P1-O2
33	j	203	PLX	C3-O4-P1-O3
33	j	203	PLX	O9-C24-O8-C5
33	n	101	PLX	O7-C6-O6-C4
33	n	101	PLX	C3-O4-P1-O1
33	n	101	PLX	C3-O4-P1-O2
33	n	101	PLX	C3-O4-P1-O3
33	n	101	PLX	C2-O1-P1-O4
33	n	101	PLX	C2-O1-P1-O2
33	n	101	PLX	C2-O1-P1-O3
33	n	101	PLX	O9-C24-C25-C26
33	r	502	PLX	O7-C6-C7-C8
33	r	502	PLX	C5-C4-O6-C6
33	r	502	PLX	O9-C24-C25-C26
34	s	402	UQ	C7-C8-C9-C10
34	s	402	UQ	C7-C8-C9-C11
34	s	402	UQ	C17-C18-C19-C21
35	w	401	ADP	PA-O3A-PB-O3B
35	w	401	ADP	C5'-O5'-PA-O1A
35	w	401	ADP	C5'-O5'-PA-O2A
31	s	401	CDL	OA9-CA7-OA8-CA6
31	s	401	CDL	C31-CA7-OA8-CA6
30	Q	101	PEE	O4-C10-O2-C2
30	l	702	PEE	O4-C10-O2-C2
31	V	201	CDL	OA7-CA5-OA6-CA4
31	r	504	CDL	OB7-CB5-OB6-CB4
31	s	401	CDL	OB7-CB5-OB6-CB4
31	V	201	CDL	C11-CA5-OA6-CA4
30	j	201	PEE	O5-C30-O3-C3
30	l	703	PEE	C2-C3-O3-C30
30	j	201	PEE	C17-C18-C19-C20
34	s	402	UQ	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
31	a	201	CDL	O1-C1-CA2-OA2
31	a	201	CDL	O1-C1-CB2-OB2
31	l	701	CDL	O1-C1-CA2-OA2
31	s	401	CDL	O1-C1-CA2-OA2
31	u	201	CDL	O1-C1-CB2-OB2
30	j	201	PEE	C31-C30-O3-C3
31	l	701	CDL	C71-CB7-OB8-CB6
31	o	201	CDL	C51-CB5-OB6-CB4
30	l	702	PEE	C31-C30-O3-C3
33	r	502	PLX	C9-C10-C11-C12
33	r	502	PLX	C11-C12-C13-C14
34	s	402	UQ	C27-C28-C29-C31
30	l	702	PEE	O5-C30-O3-C3
30	W	201	PEE	C31-C30-O3-C3
31	V	201	CDL	C31-CA7-OA8-CA6
34	s	402	UQ	C22-C23-C24-C25
31	l	701	CDL	OB9-CB7-OB8-CB6
31	k	101	CDL	C73-C74-C75-C76
31	o	201	CDL	OB7-CB5-OB6-CB4
31	V	201	CDL	CB2-C1-CA2-OA2
31	a	201	CDL	CB2-C1-CA2-OA2
31	a	201	CDL	CA2-C1-CB2-OB2
31	o	201	CDL	CA2-C1-CB2-OB2
31	r	504	CDL	CB2-C1-CA2-OA2
31	o	201	CDL	C31-CA7-OA8-CA6
31	a	201	CDL	C34-C35-C36-C37
33	g	201	PLX	C9-C10-C11-C12
33	g	201	PLX	C7-C8-C9-C10
30	U	401	PEE	C34-C35-C36-C37
31	V	201	CDL	C11-C12-C13-C14
31	V	201	CDL	C62-C63-C64-C65
31	k	101	CDL	C62-C63-C64-C65
33	g	201	PLX	C2-C1-N1-C1A
33	j	203	PLX	C13-C14-C15-C16
31	V	201	CDL	OA9-CA7-OA8-CA6
31	l	701	CDL	C71-C72-C73-C74
31	r	503	CDL	C55-C56-C57-C58
33	r	502	PLX	C7-C8-C9-C10
30	l	703	PEE	C34-C35-C36-C37
31	r	503	CDL	CB5-C51-C52-C53
31	o	201	CDL	O1-C1-CB2-OB2
31	r	503	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
31	s	401	CDL	O1-C1-CB2-OB2
31	o	201	CDL	C11-C12-C13-C14
33	j	202	PLX	C25-C26-C27-C28
32	X	201	8Q1	C6-C7-C8-C9
31	r	503	CDL	OA5-CA3-CA4-OA6
30	U	401	PEE	C31-C30-O3-C3
31	k	101	CDL	C60-C61-C62-C63
30	U	401	PEE	C17-C18-C19-C20
31	r	504	CDL	CA5-C11-C12-C13
31	r	504	CDL	CB5-C51-C52-C53
31	r	503	CDL	C58-C59-C60-C61
33	j	203	PLX	C28-C29-C30-C31
33	g	201	PLX	C2-C1-N1-C1B
31	k	101	CDL	CA7-C31-C32-C33
31	l	701	CDL	CA7-C31-C32-C33
30	r	501	PEE	C10-C11-C12-C13
31	u	201	CDL	CB7-C71-C72-C73
31	o	201	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	O1-C1-CA2-OA2
31	V	201	CDL	O1-C1-CB2-OB2
31	r	504	CDL	O1-C1-CA2-OA2
30	W	201	PEE	O5-C30-O3-C3
31	s	401	CDL	CB7-C71-C72-C73
31	s	401	CDL	C14-C15-C16-C17
30	W	201	PEE	C17-C18-C19-C20
31	a	201	CDL	CA5-C11-C12-C13
31	V	201	CDL	C56-C57-C58-C59
30	U	401	PEE	O5-C30-O3-C3
31	V	201	CDL	CA2-C1-CB2-OB2
31	l	701	CDL	CB2-C1-CA2-OA2
31	V	201	CDL	C71-CB7-OB8-CB6
30	l	703	PEE	C21-C22-C23-C24
31	o	201	CDL	C57-C58-C59-C60
31	k	101	CDL	C58-C59-C60-C61
31	o	201	CDL	C78-C79-C80-C81
31	k	101	CDL	C13-C14-C15-C16
31	r	503	CDL	CA7-C31-C32-C33
33	n	101	PLX	O8-C24-C25-C26
33	r	502	PLX	O6-C6-C7-C8
30	l	703	PEE	C11-C10-O2-C2
30	W	201	PEE	C22-C23-C24-C25
30	l	703	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	C37-C38-C39-C40
30	r	501	PEE	C37-C38-C39-C40
31	l	701	CDL	C51-C52-C53-C54
31	V	201	CDL	OB9-CB7-OB8-CB6
30	j	201	PEE	C30-C31-C32-C33
32	X	201	8Q1	C13-C14-C15-C16
33	g	201	PLX	C2-C1-N1-C1C
31	V	201	CDL	CA7-C31-C32-C33
31	s	401	CDL	C35-C36-C37-C38
30	W	201	PEE	C12-C13-C14-C15
31	o	201	CDL	C60-C61-C62-C63
31	s	401	CDL	C32-C33-C34-C35
33	g	201	PLX	C32-C33-C34-C35
33	j	202	PLX	C7-C8-C9-C10
33	n	101	PLX	C12-C13-C14-C15
31	V	201	CDL	C58-C59-C60-C61
33	j	203	PLX	C33-C34-C35-C36
33	n	101	PLX	C9-C10-C11-C12
33	e	201	PLX	O9-C24-C25-C26
33	j	202	PLX	O9-C24-C25-C26
31	V	201	CDL	C73-C74-C75-C76
31	l	701	CDL	C75-C76-C77-C78
31	o	201	CDL	C37-C38-C39-C40
31	o	201	CDL	C79-C80-C81-C82
31	r	503	CDL	C56-C57-C58-C59
31	r	503	CDL	C59-C60-C61-C62
33	r	502	PLX	C25-C26-C27-C28
33	r	502	PLX	C28-C29-C30-C31
30	W	201	PEE	C13-C14-C15-C16
30	r	501	PEE	C11-C12-C13-C14
30	r	501	PEE	C40-C41-C42-C43
31	l	701	CDL	C21-C22-C23-C24
30	Q	101	PEE	C11-C12-C13-C14
33	g	201	PLX	C33-C34-C35-C36
30	U	401	PEE	C35-C36-C37-C38
30	U	401	PEE	C13-C14-C15-C16
31	r	503	CDL	C52-C53-C54-C55
31	r	503	CDL	C74-C75-C76-C77
30	U	401	PEE	C11-C10-O2-C2
31	l	701	CDL	C51-CB5-OB6-CB4
31	r	503	CDL	C62-C63-C64-C65
31	s	401	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
33	j	203	PLX	C14-C15-C16-C17
33	j	203	PLX	C30-C31-C32-C33
31	a	201	CDL	C21-C22-C23-C24
31	a	201	CDL	C59-C60-C61-C62
30	l	702	PEE	C21-C22-C23-C24
31	V	201	CDL	C21-C22-C23-C24
31	l	701	CDL	C74-C75-C76-C77
33	g	201	PLX	C30-C31-C32-C33
33	j	203	PLX	C7-C8-C9-C10
33	r	502	PLX	C33-C34-C35-C36
30	r	501	PEE	C33-C34-C35-C36
31	V	201	CDL	C75-C76-C77-C78
31	o	201	CDL	C12-C13-C14-C15
33	r	502	PLX	C11-C10-C9-C8
31	a	201	CDL	CB7-C71-C72-C73
33	n	101	PLX	C14-C15-C16-C17
30	j	201	PEE	C22-C23-C24-C25
31	V	201	CDL	C79-C80-C81-C82
31	a	201	CDL	C81-C82-C83-C84
31	l	701	CDL	C15-C16-C17-C18
31	s	401	CDL	C75-C76-C77-C78
33	n	101	PLX	C10-C11-C12-C13
31	k	101	CDL	C55-C56-C57-C58
31	k	101	CDL	C56-C57-C58-C59
31	l	701	CDL	C72-C73-C74-C75
31	o	201	CDL	C54-C55-C56-C57
31	u	201	CDL	CB5-C51-C52-C53
30	j	201	PEE	C21-C22-C23-C24
30	l	702	PEE	C31-C32-C33-C34
31	V	201	CDL	C55-C56-C57-C58
30	U	401	PEE	C23-C24-C25-C26
31	k	101	CDL	C76-C77-C78-C79
31	r	503	CDL	C71-C72-C73-C74
31	r	503	CDL	C16-C17-C18-C19
31	r	503	CDL	C37-C38-C39-C40
33	j	202	PLX	C11-C12-C13-C14
31	o	201	CDL	C17-C18-C19-C20
31	o	201	CDL	C59-C60-C61-C62
30	l	703	PEE	C20-C21-C22-C23
31	r	503	CDL	C75-C76-C77-C78
31	r	503	CDL	CB7-C71-C72-C73
30	W	201	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	k	101	CDL	C18-C19-C20-C21
31	s	401	CDL	C37-C38-C39-C40
33	j	203	PLX	C26-C27-C28-C29
31	l	701	CDL	OB7-CB5-OB6-CB4
31	o	201	CDL	C14-C15-C16-C17
31	s	401	CDL	C71-C72-C73-C74
33	n	101	PLX	C7-C8-C9-C10
34	s	402	UQ	C18-C19-C21-C22
31	V	201	CDL	C37-C38-C39-C40
31	k	101	CDL	C35-C36-C37-C38
31	r	504	CDL	C59-C60-C61-C62
33	j	202	PLX	C18-C19-C20-C21
33	j	202	PLX	C9-C10-C11-C12
31	l	701	CDL	C73-C74-C75-C76
31	o	201	CDL	C83-C84-C85-C86
31	r	504	CDL	C17-C18-C19-C20
30	r	501	PEE	C13-C14-C15-C16
31	r	503	CDL	C31-C32-C33-C34
33	g	201	PLX	C28-C29-C30-C31
33	n	101	PLX	C11-C12-C13-C14
33	n	101	PLX	C31-C32-C33-C34
31	o	201	CDL	C76-C77-C78-C79
32	X	201	8Q1	C11-C12-C13-C14
33	j	202	PLX	C33-C34-C35-C36
30	U	401	PEE	C38-C39-C40-C41
31	a	201	CDL	C35-C36-C37-C38
31	k	101	CDL	C15-C16-C17-C18
31	k	101	CDL	C39-C40-C41-C42
33	g	201	PLX	C12-C13-C14-C15
30	W	201	PEE	C11-C10-O2-C2
30	r	501	PEE	C11-C10-O2-C2
31	V	201	CDL	C51-CB5-OB6-CB4
31	k	101	CDL	C11-CA5-OA6-CA4
31	r	503	CDL	C51-CB5-OB6-CB4
31	s	401	CDL	C11-CA5-OA6-CA4
31	s	401	CDL	CA7-C31-C32-C33
30	U	401	PEE	O4-C10-O2-C2
30	W	201	PEE	O4-C10-O2-C2
31	r	504	CDL	C56-C57-C58-C59
31	s	401	CDL	C59-C60-C61-C62
33	g	201	PLX	C11-C12-C13-C14
30	j	201	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
30	l	702	PEE	C15-C16-C17-C18
30	l	703	PEE	C15-C16-C17-C18
33	r	502	PLX	C27-C28-C29-C30
31	r	504	CDL	C74-C75-C76-C77
31	k	101	CDL	C59-C60-C61-C62
31	a	201	CDL	C71-C72-C73-C74
33	j	202	PLX	C14-C15-C16-C17
33	j	203	PLX	C27-C28-C29-C30
31	a	201	CDL	C18-C19-C20-C21
33	g	201	PLX	C13-C14-C15-C16
30	Q	101	PEE	C31-C30-O3-C3
31	a	201	CDL	C31-C32-C33-C34
30	r	501	PEE	O4-C10-O2-C2
31	V	201	CDL	OB7-CB5-OB6-CB4
31	k	101	CDL	OA7-CA5-OA6-CA4
31	s	401	CDL	OA7-CA5-OA6-CA4
31	a	201	CDL	OA5-CA3-CA4-OA6
30	W	201	PEE	C21-C22-C23-C24
31	k	101	CDL	C34-C35-C36-C37
30	l	703	PEE	C30-C31-C32-C33
31	r	503	CDL	C11-C12-C13-C14
31	r	503	CDL	C73-C74-C75-C76
31	s	401	CDL	C52-C53-C54-C55
31	o	201	CDL	OB6-CB4-CB6-OB8
31	r	503	CDL	OA6-CA4-CA6-OA8
31	V	201	CDL	C44-C45-C46-C47
33	g	201	PLX	C10-C11-C12-C13
33	g	201	PLX	C27-C28-C29-C30
30	Q	101	PEE	C10-C11-C12-C13
30	l	703	PEE	C13-C14-C15-C16
31	k	101	CDL	C14-C15-C16-C17
33	r	502	PLX	C13-C14-C15-C16
33	r	502	PLX	C30-C31-C32-C33
31	r	504	CDL	C58-C59-C60-C61
31	r	503	CDL	OB7-CB5-OB6-CB4
31	u	201	CDL	CA2-C1-CB2-OB2
31	s	401	CDL	C82-C83-C84-C85
33	n	101	PLX	C15-C16-C17-C18
31	k	101	CDL	C71-C72-C73-C74
31	l	701	CDL	C64-C65-C66-C67
31	o	201	CDL	C73-C74-C75-C76
31	V	201	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	C31-C32-C33-C34
31	k	101	CDL	C17-C18-C19-C20
33	j	202	PLX	C27-C28-C29-C30
31	r	504	CDL	C60-C61-C62-C63
31	a	201	CDL	OA5-CA3-CA4-CA6
31	o	201	CDL	OB5-CB3-CB4-CB6
31	r	503	CDL	OA5-CA3-CA4-CA6
31	s	401	CDL	OA5-CA3-CA4-CA6
33	j	202	PLX	O4-C3-C4-C5
31	o	201	CDL	C55-C56-C57-C58
33	g	201	PLX	C25-C26-C27-C28
33	j	203	PLX	C25-C26-C27-C28
30	W	201	PEE	C20-C21-C22-C23
31	r	504	CDL	CA7-C31-C32-C33
31	o	201	CDL	C11-CA5-OA6-CA4
31	r	503	CDL	C35-C36-C37-C38
31	a	201	CDL	C43-C44-C45-C46
31	k	101	CDL	C71-CB7-OB8-CB6
30	r	501	PEE	C36-C37-C38-C39
30	Q	101	PEE	C1-C2-C3-O3
30	W	201	PEE	C1-C2-C3-O3
31	V	201	CDL	CB3-CB4-CB6-OB8
31	r	504	CDL	CA3-CA4-CA6-OA8
33	e	201	PLX	C3-C4-C5-O8
31	r	503	CDL	C24-C25-C26-C27
31	k	101	CDL	C23-C24-C25-C26
30	Q	101	PEE	C35-C36-C37-C38
31	r	503	CDL	C82-C83-C84-C85
31	k	101	CDL	C75-C76-C77-C78
31	r	503	CDL	C71-CB7-OB8-CB6
31	l	701	CDL	C13-C14-C15-C16
33	n	101	PLX	C13-C14-C15-C16
30	Q	101	PEE	O5-C30-O3-C3
31	V	201	CDL	C74-C75-C76-C77
31	k	101	CDL	OB9-CB7-OB8-CB6
31	a	201	CDL	C52-C53-C54-C55
31	s	401	CDL	C34-C35-C36-C37
31	a	201	CDL	C14-C15-C16-C17
33	j	202	PLX	C30-C31-C32-C33
31	r	503	CDL	C36-C37-C38-C39
31	r	503	CDL	CA5-C11-C12-C13
31	V	201	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	C55-C56-C57-C58
33	j	202	PLX	C28-C29-C30-C31
33	j	203	PLX	C29-C30-C31-C32
33	n	101	PLX	C11-C10-C9-C8
33	n	101	PLX	C34-C35-C36-C37
31	a	201	CDL	C62-C63-C64-C65
31	r	503	CDL	C78-C79-C80-C81
30	l	702	PEE	O3P-C1-C2-O2
31	a	201	CDL	OB5-CB3-CB4-OB6
31	r	503	CDL	OB5-CB3-CB4-OB6
31	k	101	CDL	C52-C53-C54-C55
31	a	201	CDL	C11-CA5-OA6-CA4
31	r	504	CDL	C14-C15-C16-C17
32	X	201	8Q1	C11-C10-C9-C8
30	j	201	PEE	C41-C42-C43-C44
31	r	504	CDL	C71-C72-C73-C74
31	s	401	CDL	C55-C56-C57-C58
33	j	203	PLX	C9-C10-C11-C12
33	n	101	PLX	C16-C17-C18-C19
31	k	101	CDL	C11-C12-C13-C14
31	k	101	CDL	C32-C33-C34-C35
31	k	101	CDL	C41-C42-C43-C44
31	k	101	CDL	C43-C44-C45-C46
31	o	201	CDL	C75-C76-C77-C78
30	l	702	PEE	O2-C2-C3-O3
31	r	504	CDL	OA6-CA4-CA6-OA8
31	a	201	CDL	C84-C85-C86-C87
30	l	702	PEE	C32-C33-C34-C35
31	r	503	CDL	OB9-CB7-OB8-CB6
30	U	401	PEE	C44-C45-C46-C47
31	r	503	CDL	C34-C35-C36-C37
31	a	201	CDL	C31-CA7-OA8-CA6
31	r	504	CDL	C64-C65-C66-C67
30	l	702	PEE	C24-C25-C26-C27
31	l	701	CDL	C62-C63-C64-C65
31	r	503	CDL	C20-C21-C22-C23
30	r	501	PEE	C17-C18-C19-C20
31	a	201	CDL	C55-C56-C57-C58
30	Q	101	PEE	C2-C1-O3P-P
31	V	201	CDL	C1-CB2-OB2-PB2
34	s	402	UQ	C12-C13-C14-C16
31	k	101	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
31	k	101	CDL	OA5-CA3-CA4-CA6
31	l	701	CDL	OA5-CA3-CA4-CA6
31	r	504	CDL	OA5-CA3-CA4-CA6
31	o	201	CDL	C13-C14-C15-C16
33	n	101	PLX	C19-C20-C21-C22
31	V	201	CDL	C64-C65-C66-C67
33	j	202	PLX	C34-C35-C36-C37
30	l	702	PEE	C42-C43-C44-C45
31	k	101	CDL	C37-C38-C39-C40
31	s	401	CDL	C15-C16-C17-C18
33	j	202	PLX	C12-C13-C14-C15
31	a	201	CDL	C54-C55-C56-C57
31	k	101	CDL	C38-C39-C40-C41
30	l	703	PEE	C1-C2-C3-O3
30	r	501	PEE	C1-C2-C3-O3
31	o	201	CDL	CB3-CB4-CB6-OB8
31	a	201	CDL	C11-C12-C13-C14
33	n	101	PLX	C25-C26-C27-C28
31	k	101	CDL	C84-C85-C86-C87
33	j	202	PLX	C32-C33-C34-C35
33	r	502	PLX	C12-C13-C14-C15
30	l	702	PEE	C13-C14-C15-C16
33	n	101	PLX	C30-C31-C32-C33
31	o	201	CDL	C51-C52-C53-C54
33	j	202	PLX	C13-C14-C15-C16
33	g	201	PLX	C36-C37-C38-C39
31	s	401	CDL	C17-C18-C19-C20
31	s	401	CDL	C56-C57-C58-C59
30	Q	101	PEE	C30-C31-C32-C33
31	V	201	CDL	OA5-CA3-CA4-OA6
31	l	701	CDL	OA5-CA3-CA4-OA6
31	r	503	CDL	C51-C52-C53-C54
31	a	201	CDL	C51-CB5-OB6-CB4
31	o	201	CDL	C32-C33-C34-C35
31	o	201	CDL	C1-CB2-OB2-PB2
32	X	201	8Q1	O4-C1-S44-C43
30	l	703	PEE	C11-C12-C13-C14
31	a	201	CDL	C53-C54-C55-C56
31	s	401	CDL	C54-C55-C56-C57
30	U	401	PEE	O2-C2-C3-O3
31	a	201	CDL	OB6-CB4-CB6-OB8
31	s	401	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
33	j	203	PLX	C12-C13-C14-C15
30	r	501	PEE	C38-C39-C40-C41
33	j	203	PLX	O6-C6-C7-C8
33	r	502	PLX	O8-C24-C25-C26
31	r	503	CDL	C12-C13-C14-C15
31	r	504	CDL	C62-C63-C64-C65
31	V	201	CDL	C57-C58-C59-C60
34	s	402	UQ	C14-C16-C17-C18
31	s	401	CDL	C12-C13-C14-C15
32	X	201	8Q1	C6-C1-S44-C43
31	s	401	CDL	CB2-C1-CA2-OA2
33	n	101	PLX	C35-C36-C37-C38
31	r	504	CDL	C71-CB7-OB8-CB6
33	r	502	PLX	C16-C17-C18-C19
30	l	702	PEE	O3P-C1-C2-C3
31	l	701	CDL	OB5-CB3-CB4-CB6
30	r	501	PEE	C21-C22-C23-C24
33	j	202	PLX	C24-C25-C26-C27
33	j	203	PLX	C24-C25-C26-C27
31	l	701	CDL	C31-C32-C33-C34
31	r	504	CDL	C51-C52-C53-C54
31	o	201	CDL	OA7-CA5-OA6-CA4
31	r	504	CDL	C15-C16-C17-C18
31	r	504	CDL	C52-C53-C54-C55
30	U	401	PEE	C39-C40-C41-C42
30	j	201	PEE	C35-C36-C37-C38
30	r	501	PEE	C39-C40-C41-C42
33	g	201	PLX	C14-C15-C16-C17
33	r	502	PLX	C14-C15-C16-C17
31	a	201	CDL	OA9-CA7-OA8-CA6
30	r	501	PEE	C12-C13-C14-C15
30	U	401	PEE	O3P-C1-C2-O2
31	l	701	CDL	OB5-CB3-CB4-OB6
31	r	504	CDL	OA5-CA3-CA4-OA6
33	e	201	PLX	O4-C3-C4-O6
31	l	701	CDL	C16-C17-C18-C19
31	r	503	CDL	CA3-CA4-CA6-OA8
31	a	201	CDL	C17-C18-C19-C20
30	l	703	PEE	C5-C4-O4P-P
30	j	201	PEE	C11-C12-C13-C14
31	a	201	CDL	C72-C73-C74-C75
30	W	201	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	a	201	CDL	OA7-CA5-OA6-CA4
31	r	504	CDL	OB9-CB7-OB8-CB6
31	s	401	CDL	C84-C85-C86-C87
31	r	504	CDL	C11-C12-C13-C14
31	u	201	CDL	C72-C73-C74-C75
33	n	101	PLX	C28-C29-C30-C31
33	e	201	PLX	C29-C30-C31-C32
31	l	701	CDL	C56-C57-C58-C59
31	k	101	CDL	CB2-C1-CA2-OA2
30	r	501	PEE	C30-C31-C32-C33
30	r	501	PEE	C14-C15-C16-C17
31	o	201	CDL	C84-C85-C86-C87
31	a	201	CDL	CB5-C51-C52-C53
33	n	101	PLX	C25-C24-O8-C5
31	o	201	CDL	C64-C65-C66-C67
31	V	201	CDL	CB5-C51-C52-C53
33	r	502	PLX	C31-C32-C33-C34
30	U	401	PEE	O3P-C1-C2-C3
31	V	201	CDL	OA5-CA3-CA4-CA6
33	e	201	PLX	O4-C3-C4-C5
31	a	201	CDL	OB7-CB5-OB6-CB4
31	V	201	CDL	C78-C79-C80-C81
31	s	401	CDL	C57-C58-C59-C60
33	j	203	PLX	C11-C10-C9-C8
31	s	401	CDL	CA5-C11-C12-C13
31	l	701	CDL	C53-C54-C55-C56
33	n	101	PLX	C27-C28-C29-C30
30	j	201	PEE	C36-C37-C38-C39
30	Q	101	PEE	C24-C25-C26-C27
31	a	201	CDL	C15-C16-C17-C18
31	V	201	CDL	C32-C33-C34-C35
31	a	201	CDL	C75-C76-C77-C78
31	r	504	CDL	C13-C14-C15-C16
33	j	202	PLX	O4-C3-C4-O6
30	j	201	PEE	C12-C13-C14-C15
33	n	101	PLX	C29-C30-C31-C32
31	o	201	CDL	C72-C73-C74-C75
30	Q	101	PEE	O2-C2-C3-O3
30	r	501	PEE	O2-C2-C3-O3
31	V	201	CDL	OA6-CA4-CA6-OA8
33	e	201	PLX	O6-C4-C5-O8
33	r	502	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
31	r	503	CDL	CB2-C1-CA2-OA2
31	u	201	CDL	C73-C74-C75-C76
30	j	201	PEE	C32-C33-C34-C35
31	s	401	CDL	CB3-CB4-CB6-OB8
31	a	201	CDL	C12-C13-C14-C15
30	j	201	PEE	C23-C24-C25-C26
30	j	201	PEE	C38-C39-C40-C41
31	r	503	CDL	C40-C41-C42-C43
30	Q	101	PEE	C1-O3P-P-O1P
30	Q	101	PEE	C4-O4P-P-O3P
30	l	703	PEE	C4-O4P-P-O1P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C1-O3P-P-O4P
31	V	201	CDL	CB2-OB2-PB2-OB4
31	V	201	CDL	CB2-OB2-PB2-OB5
31	V	201	CDL	CB3-OB5-PB2-OB2
31	a	201	CDL	CA2-OA2-PA1-OA4
31	a	201	CDL	CB2-OB2-PB2-OB4
31	a	201	CDL	CB2-OB2-PB2-OB5
31	k	101	CDL	CA2-OA2-PA1-OA3
31	k	101	CDL	CA2-OA2-PA1-OA4
31	k	101	CDL	CA2-OA2-PA1-OA5
31	k	101	CDL	CB2-OB2-PB2-OB4
31	o	201	CDL	CA3-OA5-PA1-OA2
31	o	201	CDL	CA3-OA5-PA1-OA3
31	o	201	CDL	CA3-OA5-PA1-OA4
31	o	201	CDL	CB2-OB2-PB2-OB3
31	r	503	CDL	CA2-OA2-PA1-OA3
31	r	503	CDL	CB2-OB2-PB2-OB5
31	r	503	CDL	CB3-OB5-PB2-OB2
31	r	503	CDL	CB3-OB5-PB2-OB4
31	r	504	CDL	CA3-OA5-PA1-OA3
31	r	504	CDL	CB2-OB2-PB2-OB3
31	r	504	CDL	CB2-OB2-PB2-OB5
31	u	201	CDL	CA2-OA2-PA1-OA4
31	u	201	CDL	CA3-OA5-PA1-OA3
31	u	201	CDL	CB2-OB2-PB2-OB3
33	e	201	PLX	C3-O4-P1-O3
33	g	201	PLX	C3-O4-P1-O3
33	n	101	PLX	C5-C4-O6-C6
33	r	502	PLX	C2-O1-P1-O3
35	w	401	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
31	r	503	CDL	C81-C82-C83-C84
31	o	201	CDL	C34-C35-C36-C37
31	V	201	CDL	C32-C31-CA7-OA8
30	Q	101	PEE	C38-C39-C40-C41
30	j	201	PEE	C1-C2-O2-C10
31	k	101	CDL	CA6-CA4-OA6-CA5
31	k	101	CDL	C44-C45-C46-C47
31	a	201	CDL	OB5-CB3-CB4-CB6
31	r	503	CDL	OB5-CB3-CB4-CB6
31	a	201	CDL	C32-C33-C34-C35
31	a	201	CDL	C74-C75-C76-C77
32	X	201	8Q1	C10-C11-C12-C13
34	s	402	UQ	C17-C18-C19-C20
30	l	703	PEE	O2-C2-C3-O3
31	s	401	CDL	C83-C84-C85-C86
31	a	201	CDL	C23-C24-C25-C26
33	g	201	PLX	C35-C36-C37-C38
31	r	504	CDL	C72-C71-CB7-OB8
34	s	402	UQ	C9-C11-C12-C13
31	V	201	CDL	C59-C60-C61-C62
30	Q	101	PEE	C34-C35-C36-C37
31	k	101	CDL	C64-C65-C66-C67
33	g	201	PLX	C6-C7-C8-C9
31	k	101	CDL	C36-C37-C38-C39
31	k	101	CDL	C82-C83-C84-C85
30	j	201	PEE	C40-C41-C42-C43
31	k	101	CDL	C16-C17-C18-C19
31	s	401	CDL	C60-C61-C62-C63
30	r	501	PEE	C20-C21-C22-C23
30	r	501	PEE	C43-C44-C45-C46
31	o	201	CDL	CA7-C31-C32-C33
31	k	101	CDL	OB6-CB4-CB6-OB8
31	r	503	CDL	C42-C43-C44-C45
31	u	201	CDL	C1-CB2-OB2-PB2
31	r	503	CDL	C18-C19-C20-C21
31	l	701	CDL	C59-C60-C61-C62
31	o	201	CDL	C36-C37-C38-C39
30	l	703	PEE	C38-C39-C40-C41
33	r	502	PLX	C3-C4-C5-O8
31	a	201	CDL	C39-C40-C41-C42
31	a	201	CDL	C36-C37-C38-C39
33	r	502	PLX	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C11-C10-C9-C8
31	a	201	CDL	C38-C39-C40-C41
30	Q	101	PEE	C21-C22-C23-C24
33	j	203	PLX	C34-C35-C36-C37
34	s	402	UQ	C13-C14-C16-C17
31	s	401	CDL	C77-C78-C79-C80
31	l	701	CDL	C18-C19-C20-C21
30	W	201	PEE	C16-C17-C18-C19
33	j	203	PLX	C19-C20-C21-C22
30	l	703	PEE	C2-C1-O3P-P
30	j	201	PEE	C14-C15-C16-C17
31	k	101	CDL	C21-C22-C23-C24
30	Q	101	PEE	C23-C24-C25-C26
31	l	701	CDL	C82-C83-C84-C85
33	e	201	PLX	C35-C36-C37-C38
31	o	201	CDL	C35-C36-C37-C38
30	Q	101	PEE	C39-C40-C41-C42
33	e	201	PLX	C30-C31-C32-C33
31	o	201	CDL	C77-C78-C79-C80
33	e	201	PLX	O8-C24-C25-C26
31	r	503	CDL	C23-C24-C25-C26
30	l	702	PEE	C2-C1-O3P-P
30	U	401	PEE	C42-C43-C44-C45
31	u	201	CDL	C55-C56-C57-C58
30	r	501	PEE	C34-C35-C36-C37
30	U	401	PEE	C1-C2-C3-O3
30	l	702	PEE	C1-C2-C3-O3
31	V	201	CDL	CA3-CA4-CA6-OA8
33	r	502	PLX	C19-C20-C21-C22
33	j	203	PLX	O9-C24-C25-C26
33	e	201	PLX	C28-C29-C30-C31
30	U	401	PEE	C11-C12-C13-C14
33	j	203	PLX	O4-C3-C4-O6
30	W	201	PEE	C23-C24-C25-C26
30	l	702	PEE	C38-C39-C40-C41
31	r	504	CDL	C16-C17-C18-C19
34	s	402	UQ	C23-C24-C26-C27
30	U	401	PEE	C2-C1-O3P-P
31	o	201	CDL	C15-C16-C17-C18
30	j	201	PEE	C16-C17-C18-C19
30	l	702	PEE	C36-C37-C38-C39
32	X	201	8Q1	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	C61-C62-C63-C64
30	l	702	PEE	C11-C12-C13-C14
30	Q	101	PEE	C14-C15-C16-C17
30	Q	101	PEE	C18-C19-C20-C21
31	o	201	CDL	C81-C82-C83-C84
33	j	203	PLX	C32-C33-C34-C35
30	r	501	PEE	O3P-C1-C2-O2
31	o	201	CDL	OA5-CA3-CA4-OA6
31	a	201	CDL	CB3-CB4-CB6-OB8
30	r	501	PEE	C31-C32-C33-C34
30	Q	101	PEE	C32-C33-C34-C35
31	o	201	CDL	C43-C44-C45-C46
33	j	202	PLX	O6-C4-C5-O8
30	U	401	PEE	C18-C19-C20-C21
30	l	702	PEE	C18-C19-C20-C21
31	o	201	CDL	C52-C51-CB5-OB6
31	u	201	CDL	C57-C58-C59-C60
30	W	201	PEE	C33-C34-C35-C36
31	l	701	CDL	C11-C12-C13-C14
30	U	401	PEE	C16-C17-C18-C19
31	a	201	CDL	CA4-CA3-OA5-PA1
33	g	201	PLX	C16-C17-C18-C19
35	w	401	ADP	PB-O3A-PA-O2A
31	l	701	CDL	C32-C31-CA7-OA8
31	s	401	CDL	C18-C19-C20-C21
30	r	501	PEE	C41-C42-C43-C44
33	e	201	PLX	C6-C7-C8-C9
31	l	701	CDL	C22-C23-C24-C25
31	a	201	CDL	C37-C38-C39-C40
30	r	501	PEE	C15-C16-C17-C18
31	a	201	CDL	C83-C84-C85-C86
31	k	101	CDL	O1-C1-CA2-OA2
33	j	203	PLX	C25-C24-O8-C5
31	r	503	CDL	C54-C55-C56-C57
31	a	201	CDL	C57-C58-C59-C60
31	r	504	CDL	OB6-CB4-CB6-OB8
30	l	702	PEE	C40-C41-C42-C43
31	o	201	CDL	C40-C41-C42-C43
31	V	201	CDL	C33-C34-C35-C36
31	a	201	CDL	C19-C20-C21-C22
31	r	504	CDL	C21-C22-C23-C24
33	j	202	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	CA4-CA3-OA5-PA1
33	j	202	PLX	O8-C24-C25-C26
30	W	201	PEE	C18-C19-C20-C21
30	U	401	PEE	C12-C13-C14-C15
31	l	701	CDL	C52-C53-C54-C55
31	a	201	CDL	C41-C42-C43-C44
31	k	101	CDL	O1-C1-CB2-OB2
31	o	201	CDL	C52-C51-CB5-OB7
31	r	504	CDL	C52-C51-CB5-OB6
33	e	201	PLX	O9-C24-O8-C5
30	U	401	PEE	C20-C21-C22-C23
33	j	202	PLX	C4-C5-O8-C24
33	e	201	PLX	C24-C25-C26-C27
31	l	701	CDL	C32-C31-CA7-OA9
31	k	101	CDL	CB3-CB4-CB6-OB8
33	j	202	PLX	C3-C4-C5-O8
31	s	401	CDL	C40-C41-C42-C43
31	l	701	CDL	C72-C71-CB7-OB8
30	r	501	PEE	O2-C10-C11-C12
31	l	701	CDL	C57-C58-C59-C60
30	j	201	PEE	O2-C10-C11-C12
30	j	201	PEE	O3-C30-C31-C32
31	a	201	CDL	C72-C71-CB7-OB8
31	V	201	CDL	C35-C36-C37-C38
30	Q	101	PEE	C16-C17-C18-C19
31	s	401	CDL	C11-C12-C13-C14
31	V	201	CDL	C72-C71-CB7-OB8
31	r	504	CDL	C12-C11-CA5-OA6
31	s	401	CDL	C72-C71-CB7-OB8
31	r	504	CDL	C52-C51-CB5-OB7

There are no ring outliers.

24 monomers are involved in 155 short contacts:

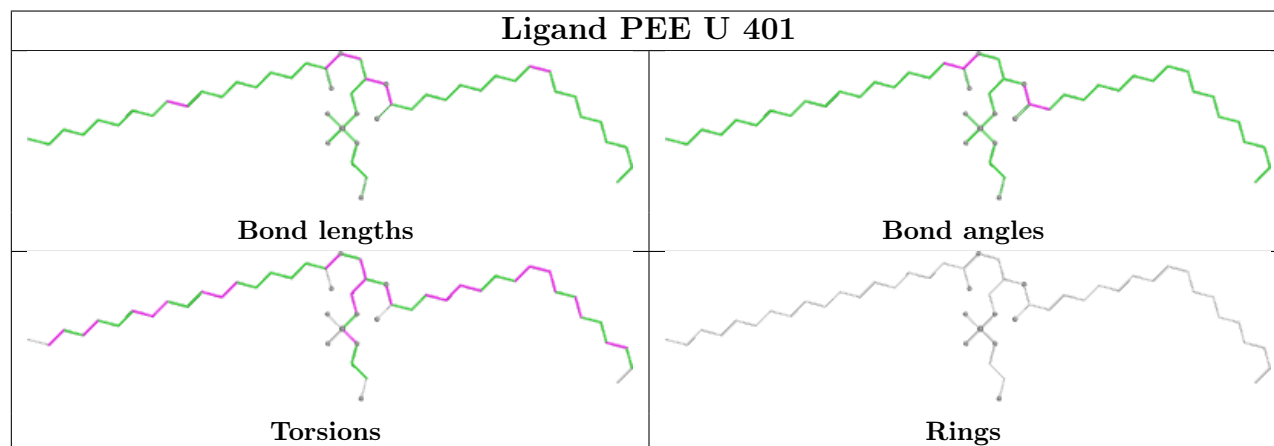
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	U	401	PEE	2	0
30	Q	101	PEE	15	0
30	l	703	PEE	7	0
30	l	702	PEE	5	0
31	o	201	CDL	6	0
34	s	402	UQ	2	0
31	r	503	CDL	14	0

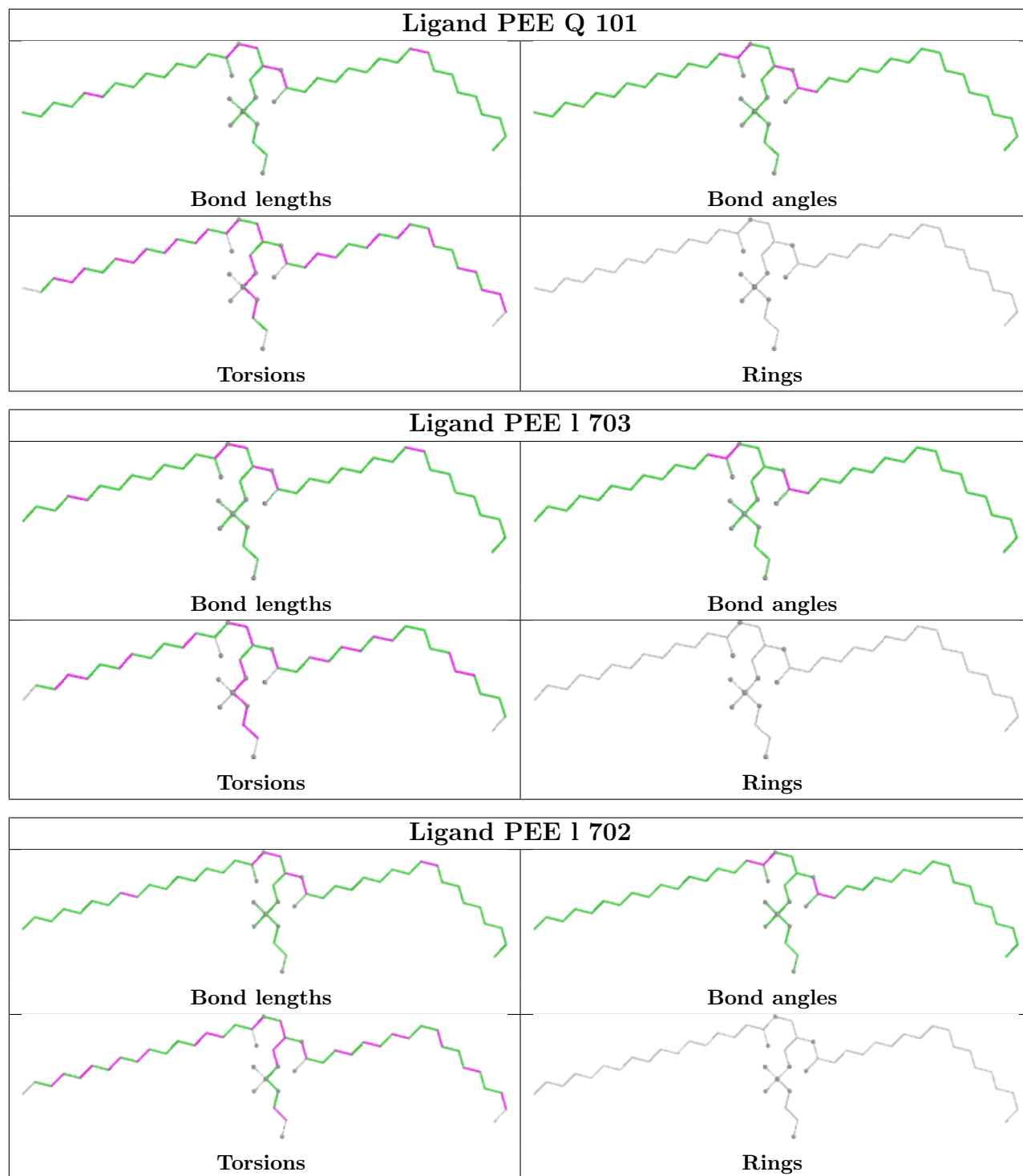
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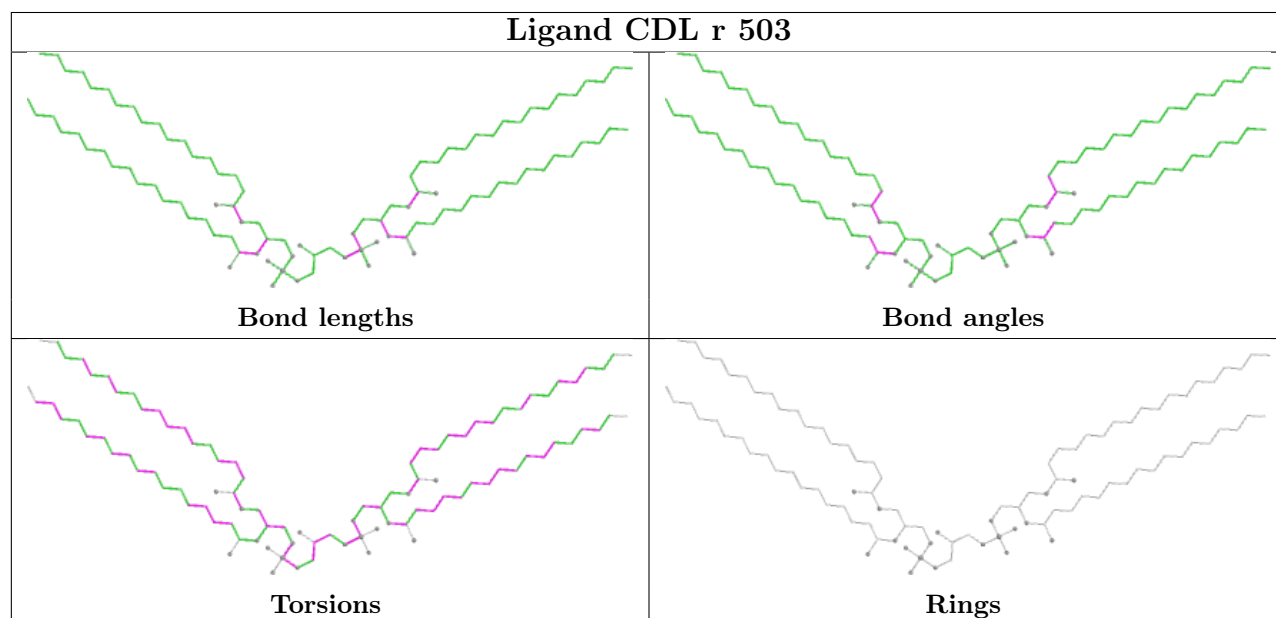
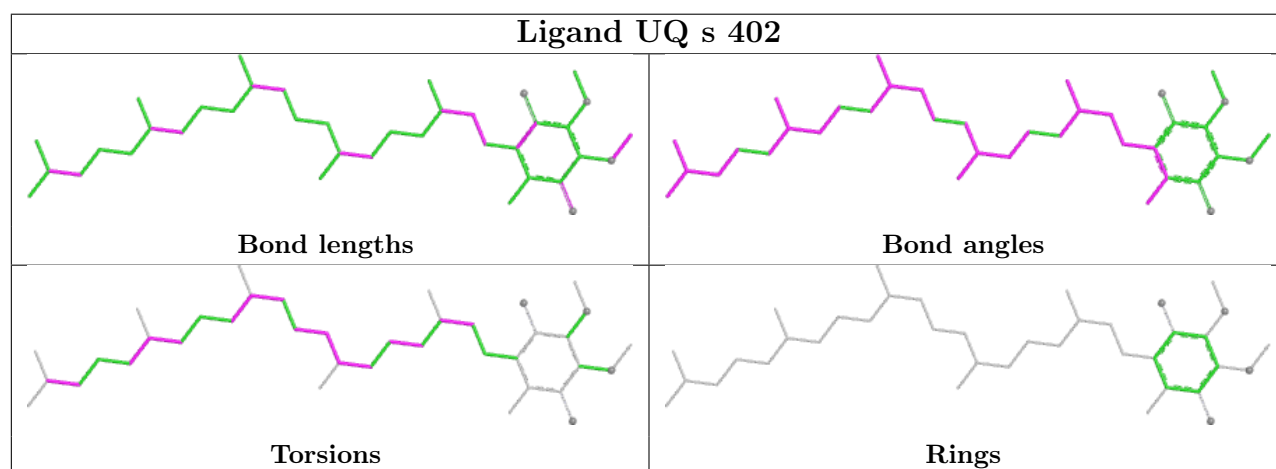
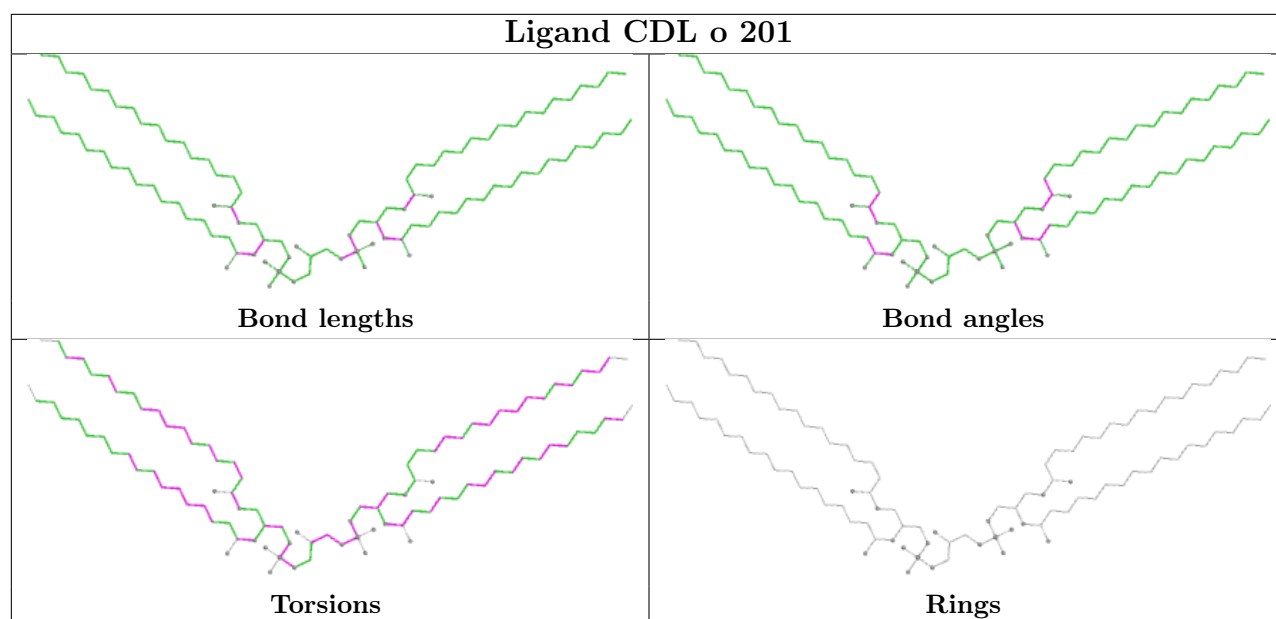
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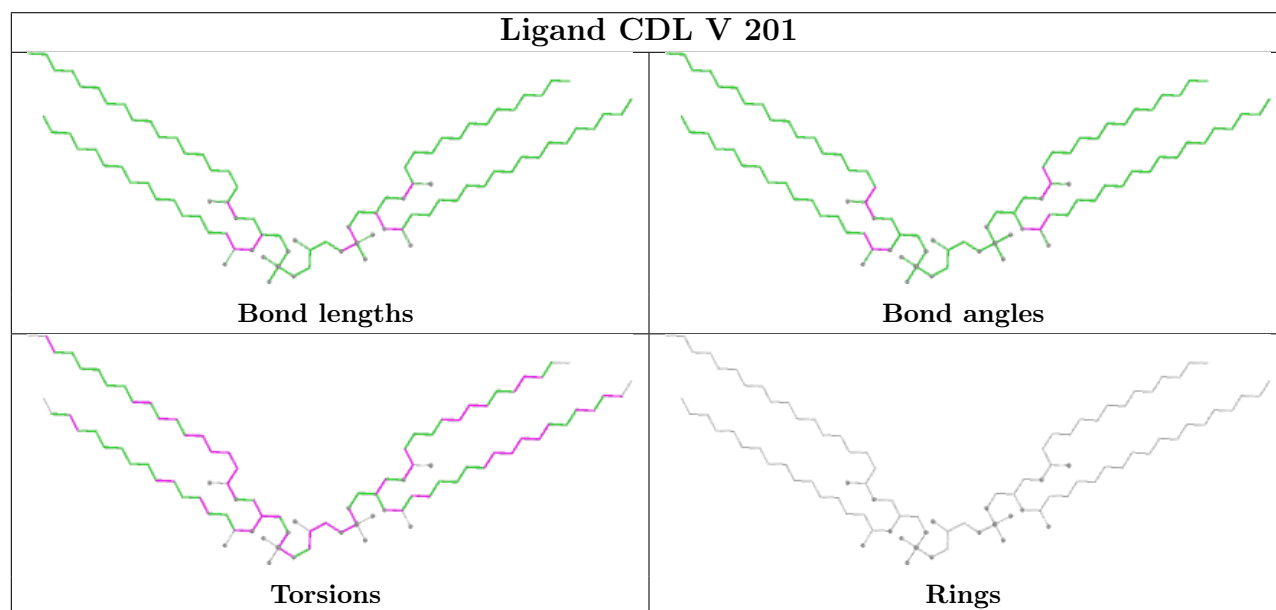
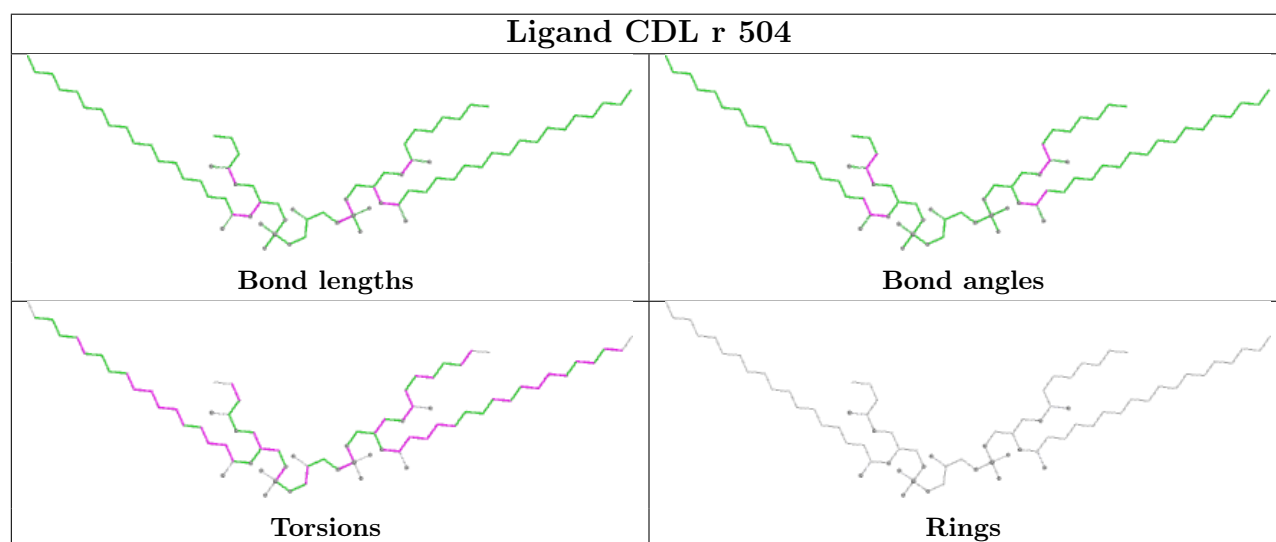
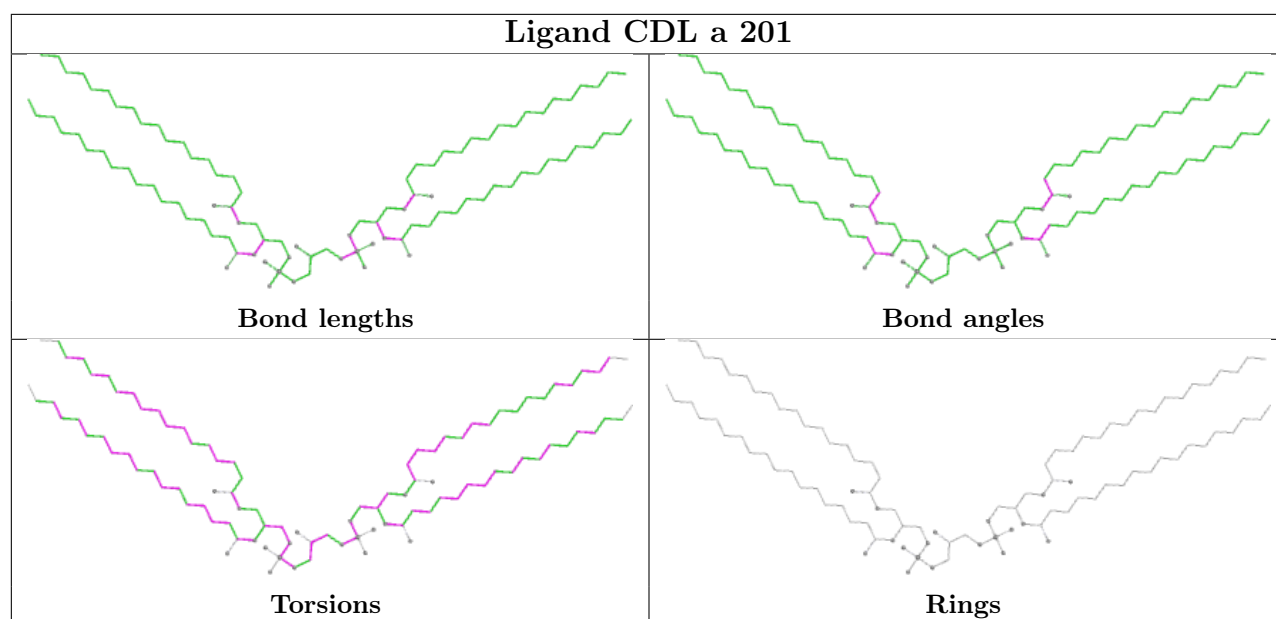
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	201	CDL	8	0
31	r	504	CDL	6	0
31	V	201	CDL	6	0
31	k	101	CDL	8	0
33	j	203	PLX	4	0
33	n	101	PLX	3	0
31	l	701	CDL	5	0
33	j	202	PLX	3	0
31	u	201	CDL	7	0
33	e	201	PLX	15	0
30	j	201	PEE	11	0
33	r	502	PLX	6	0
30	W	201	PEE	3	0
30	r	501	PEE	11	0
35	w	401	ADP	4	0
31	s	401	CDL	5	0
33	g	201	PLX	9	0

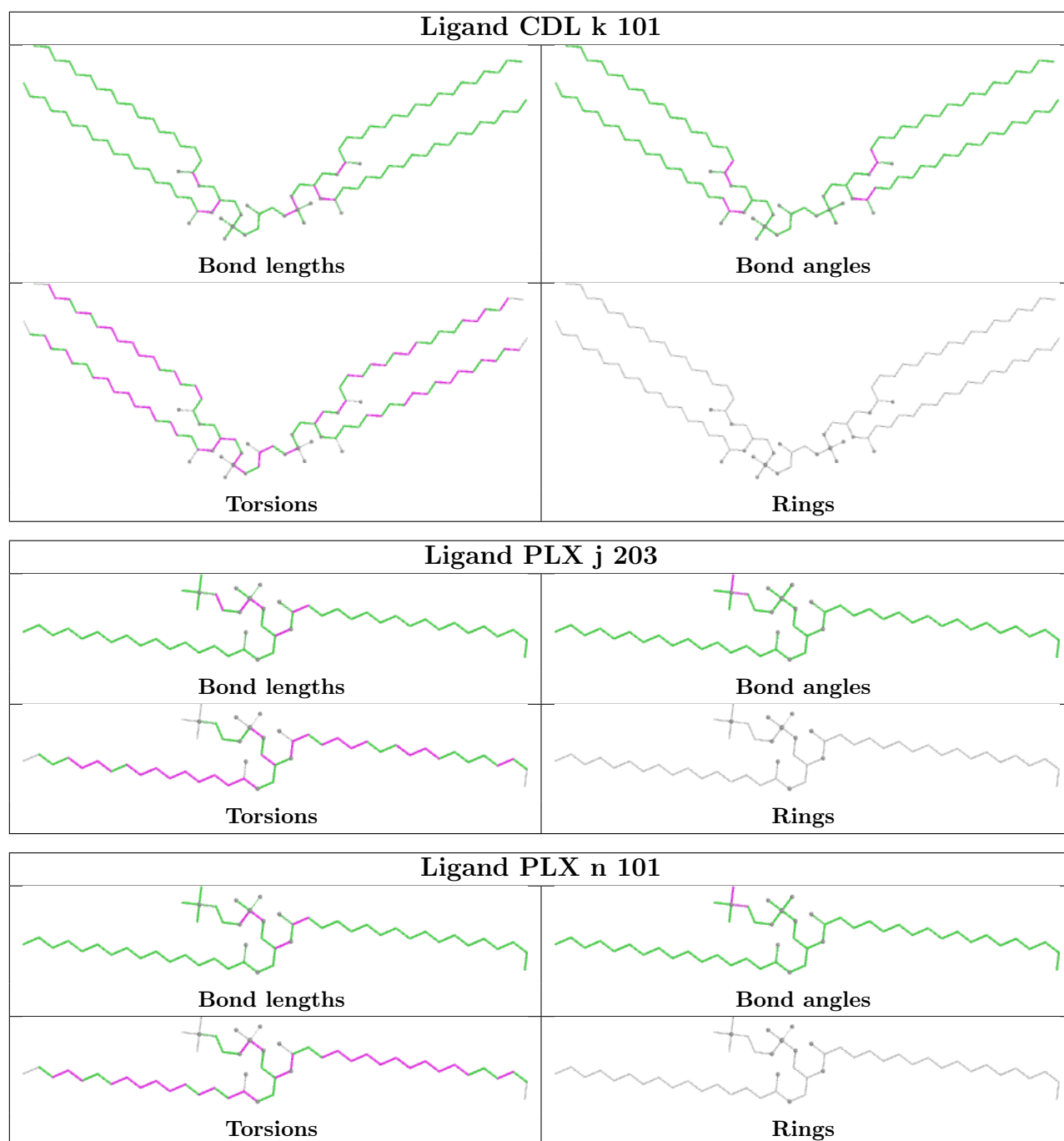
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

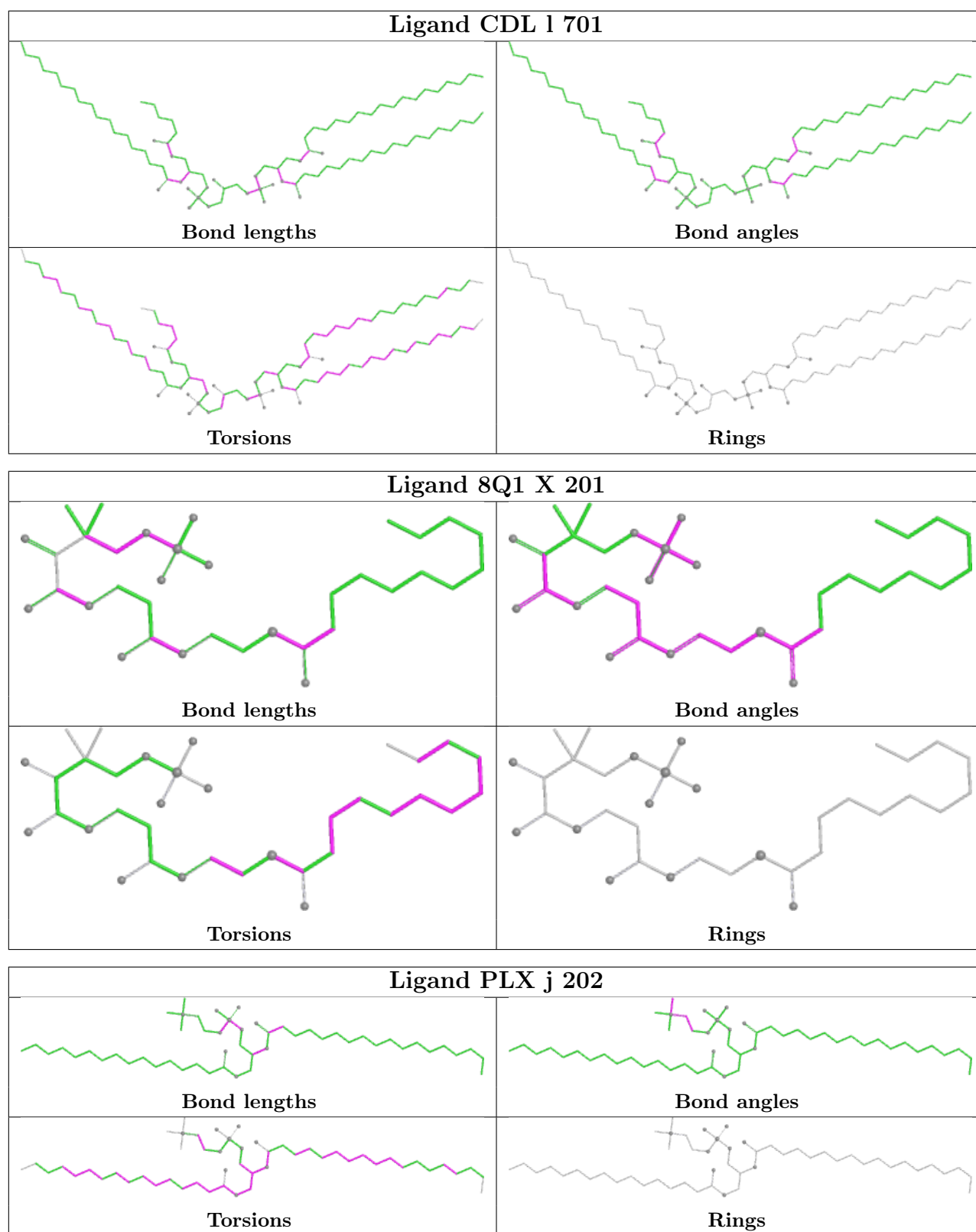


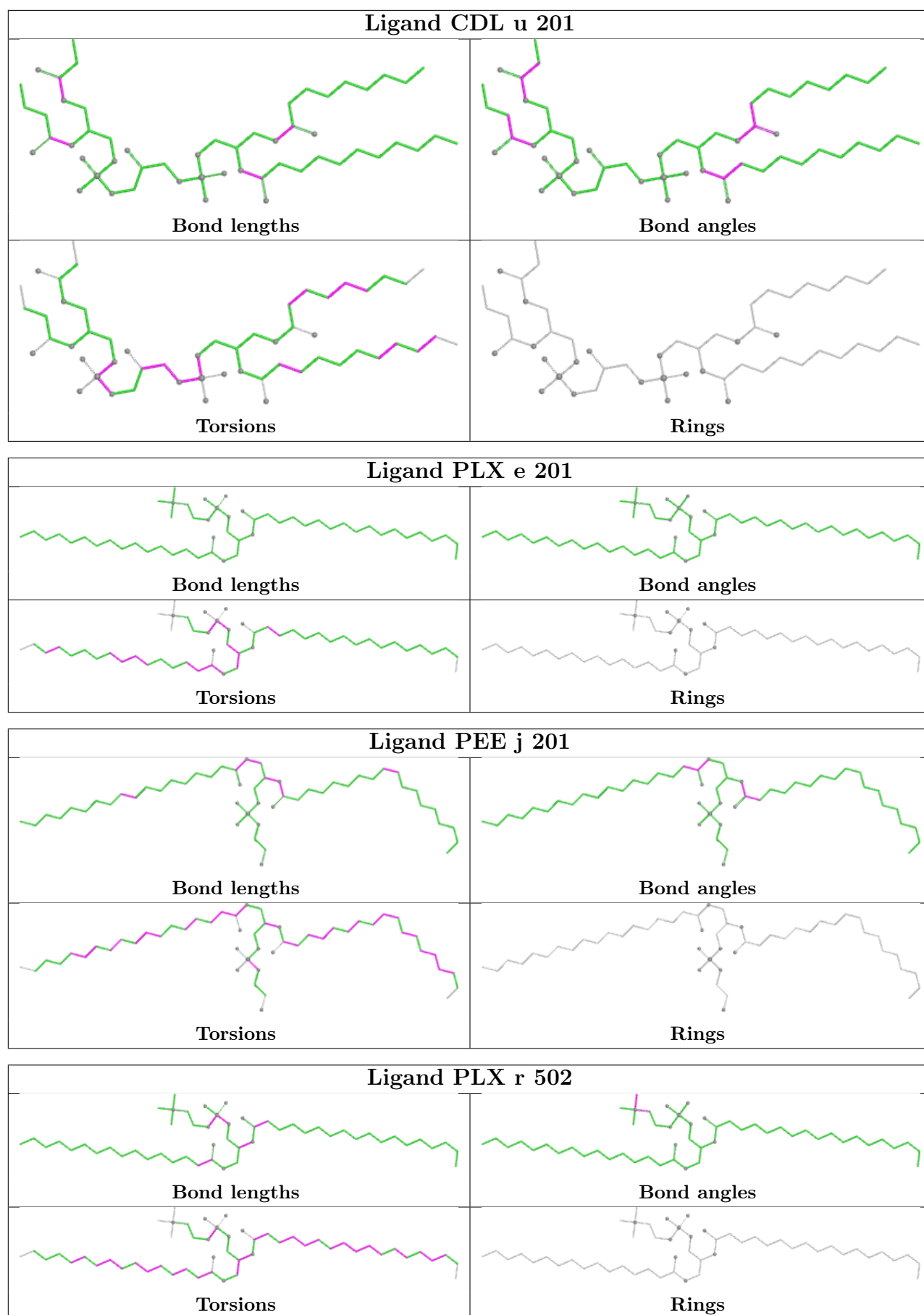


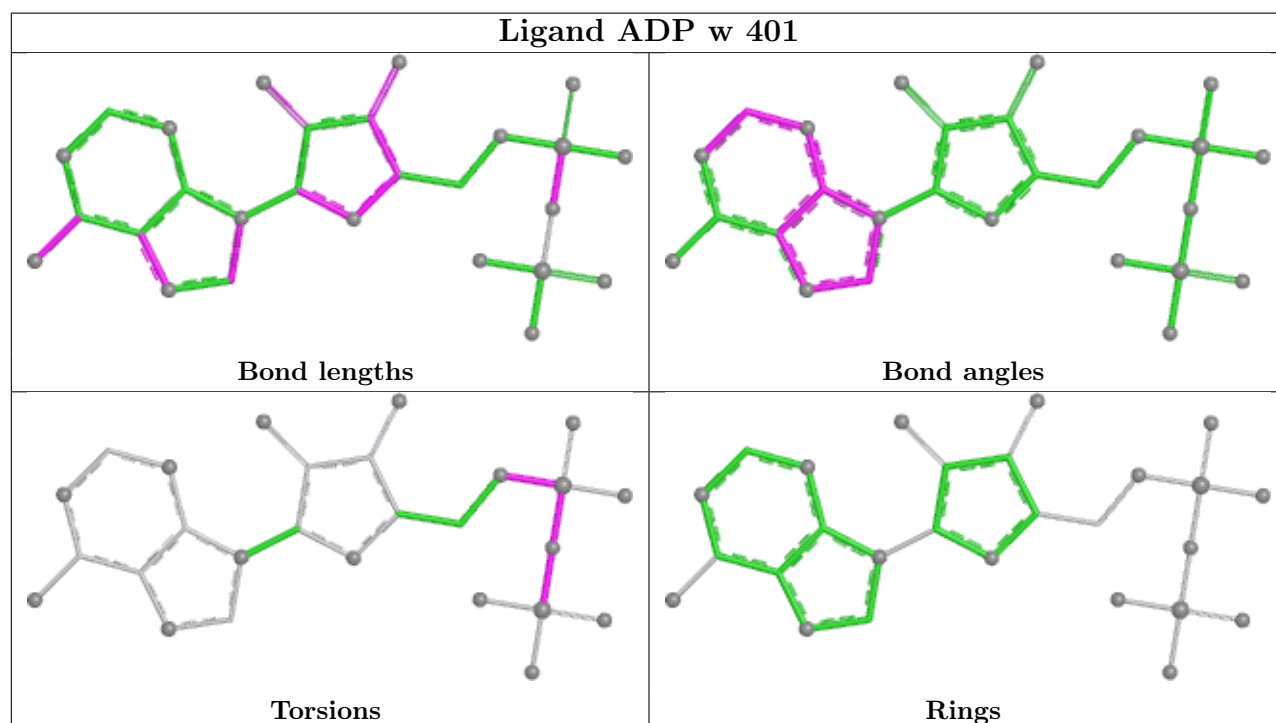
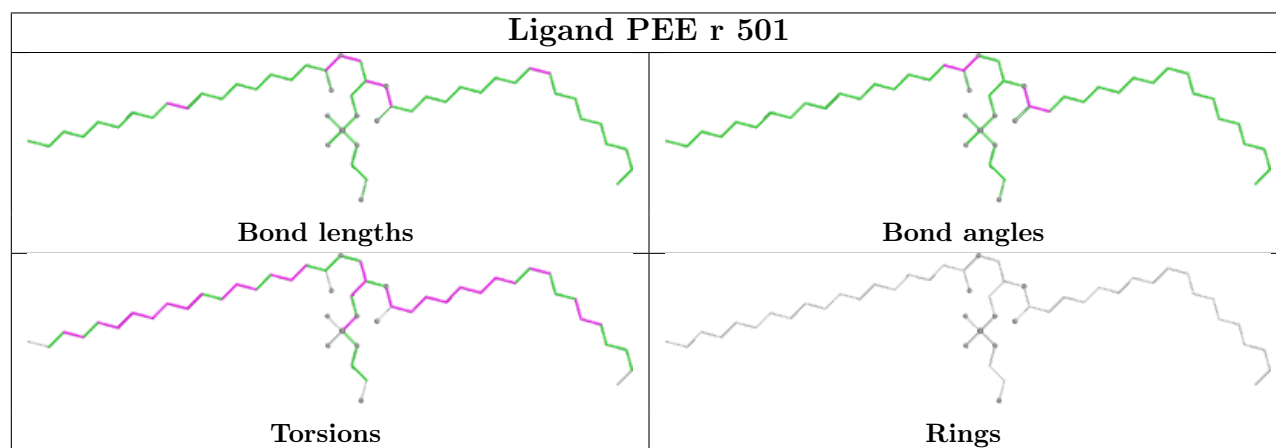
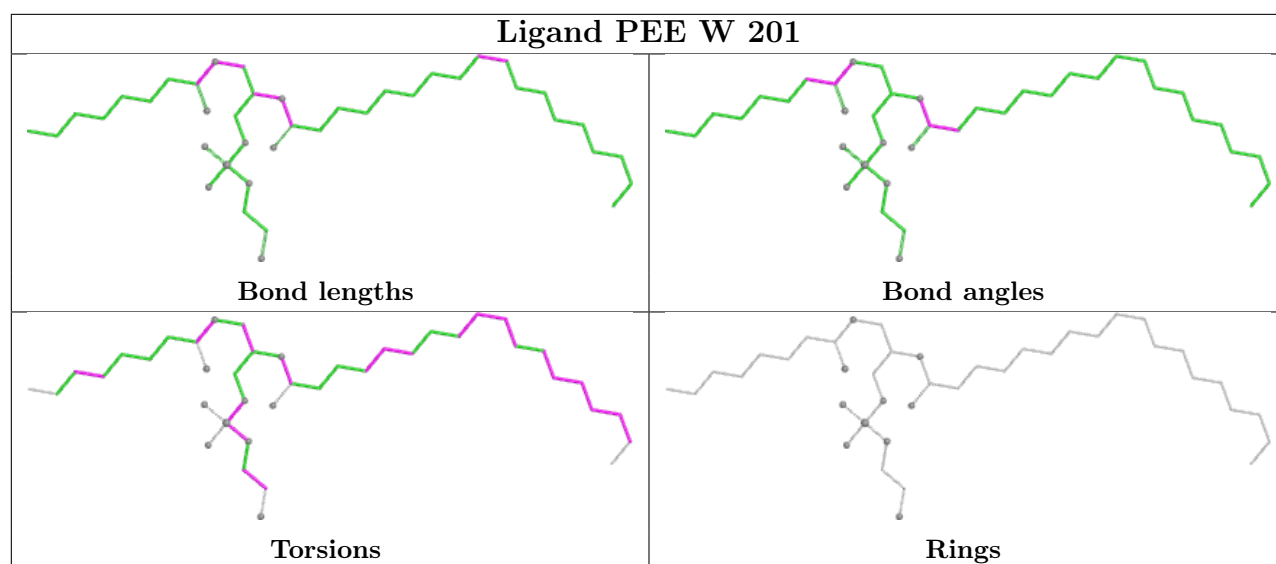


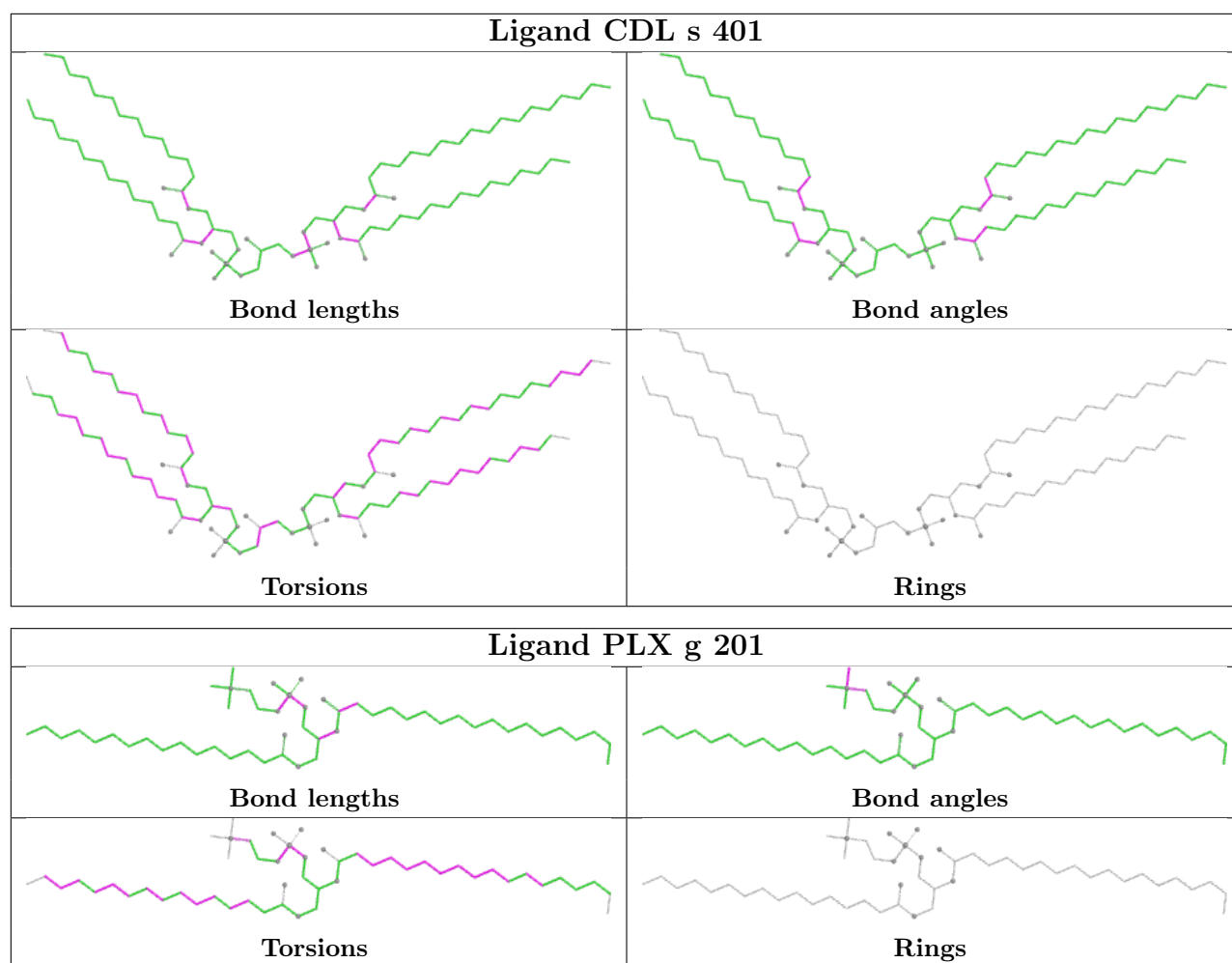












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

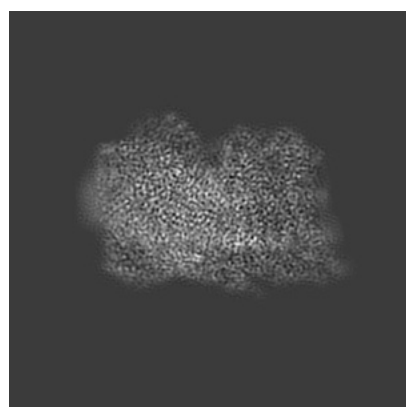
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31887. These allow visual inspection of the internal detail of the map and identification of artifacts.

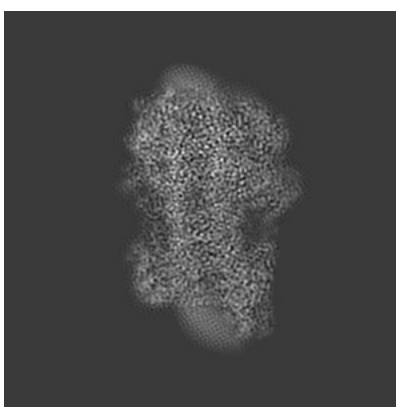
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

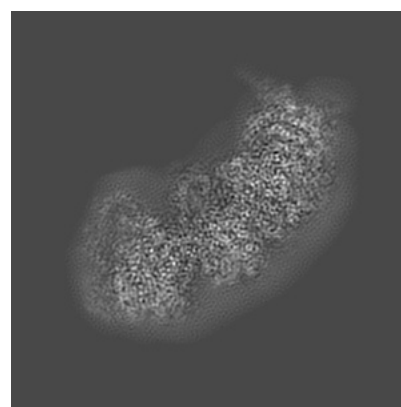
6.1.1 Primary map



X



Y

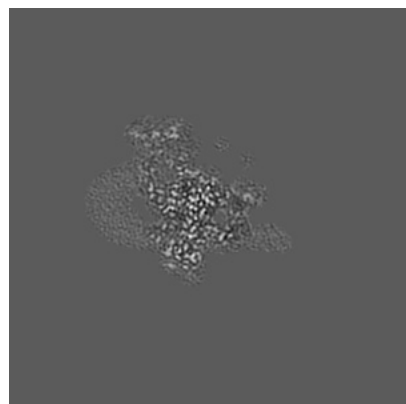


Z

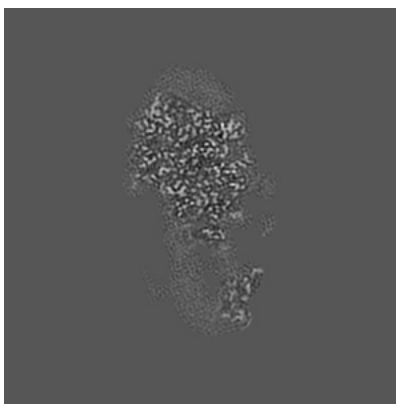
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

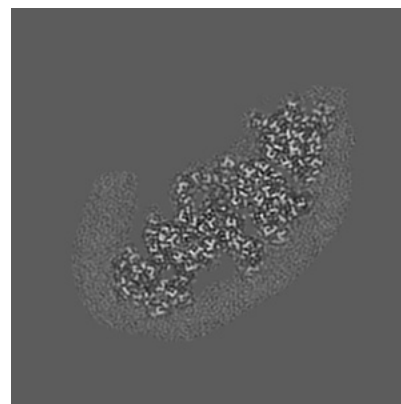
6.2.1 Primary map



X Index: 256



Y Index: 256

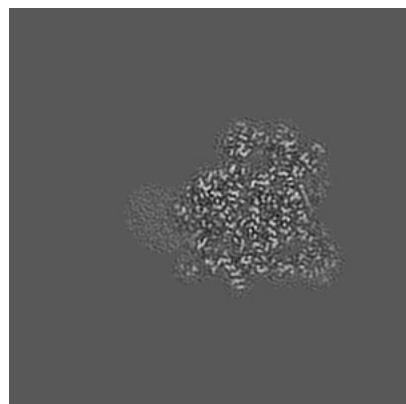


Z Index: 256

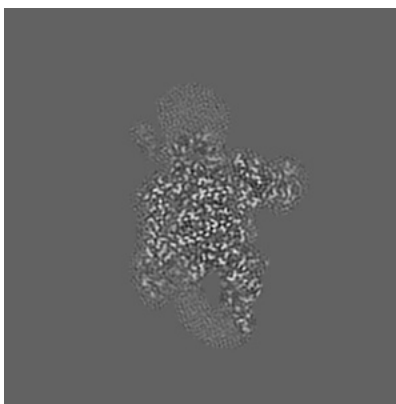
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

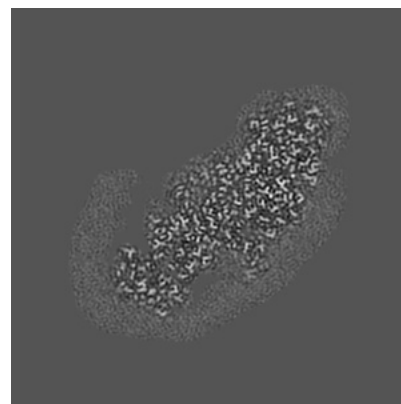
6.3.1 Primary map



X Index: 347



Y Index: 217

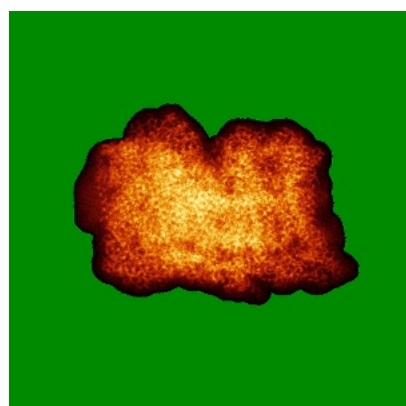


Z Index: 267

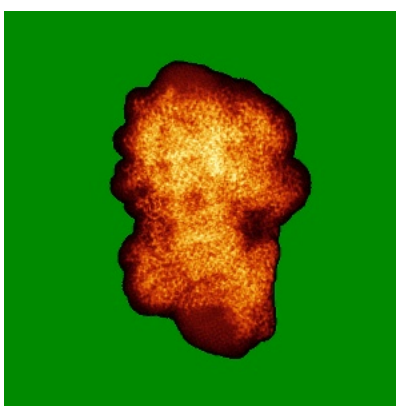
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

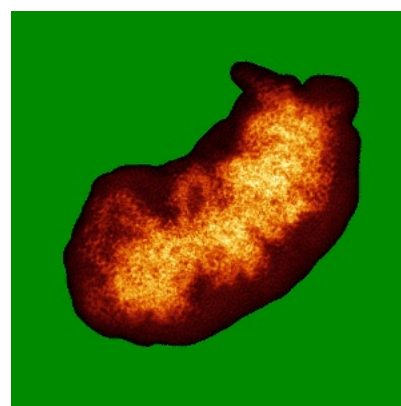
6.4.1 Primary map



X



Y

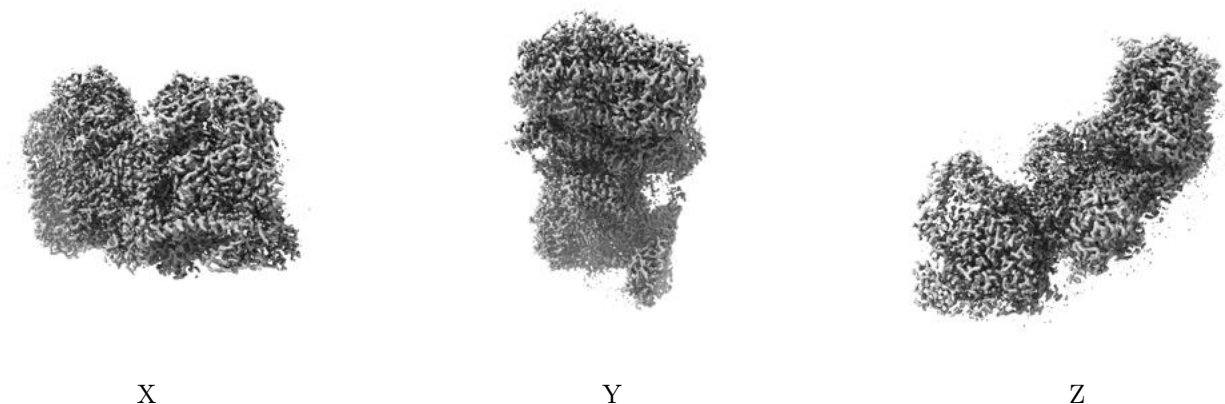


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

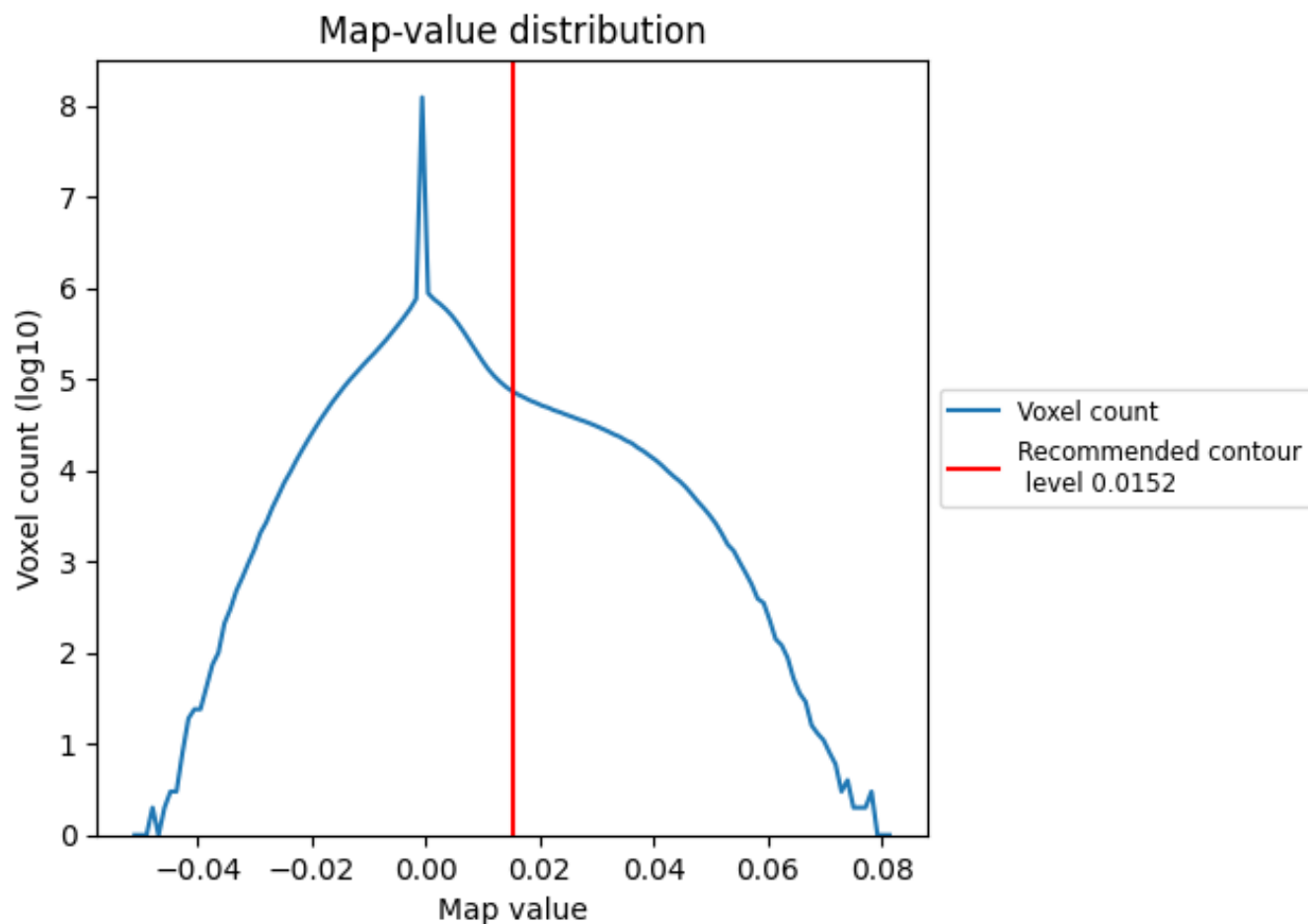
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

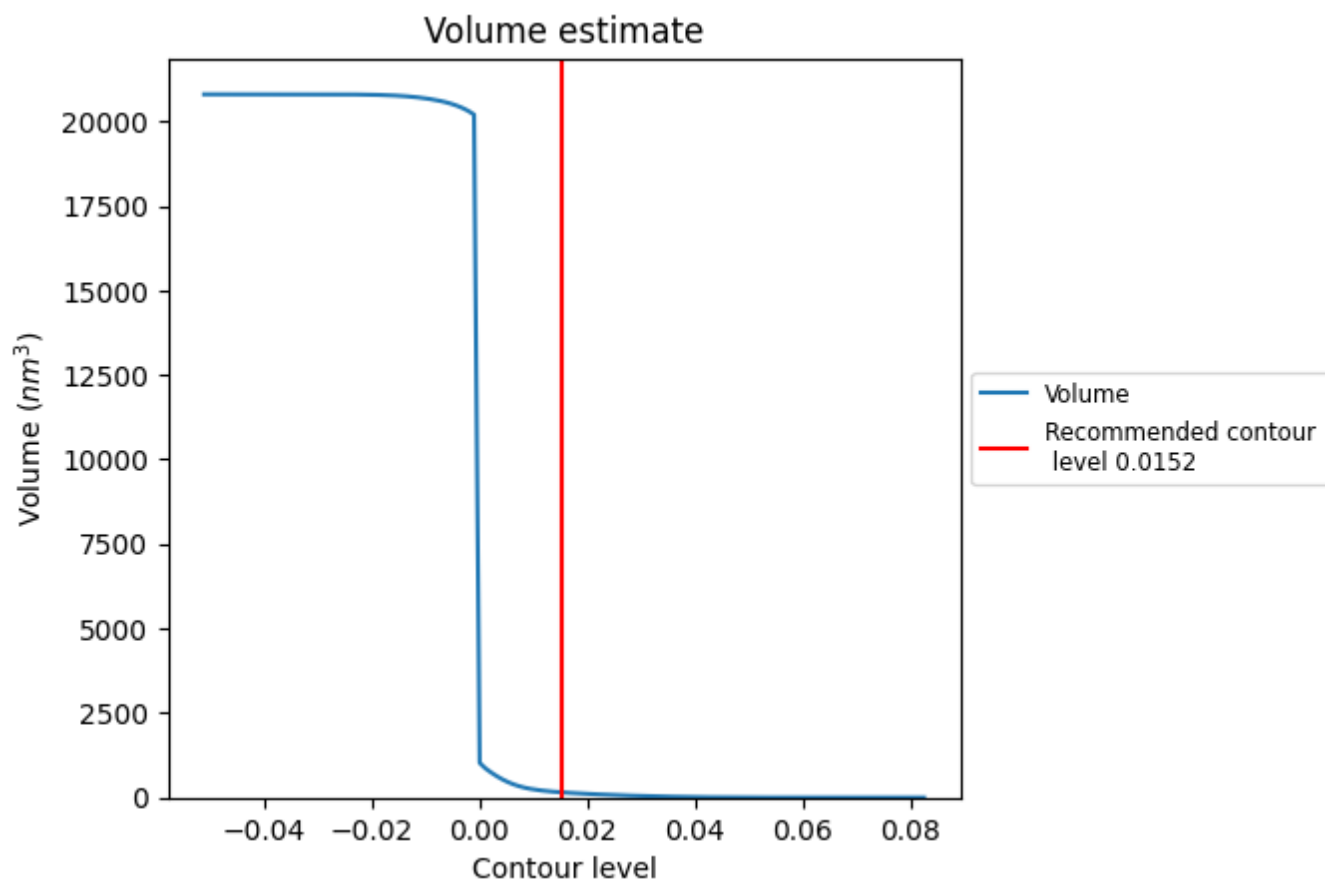
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

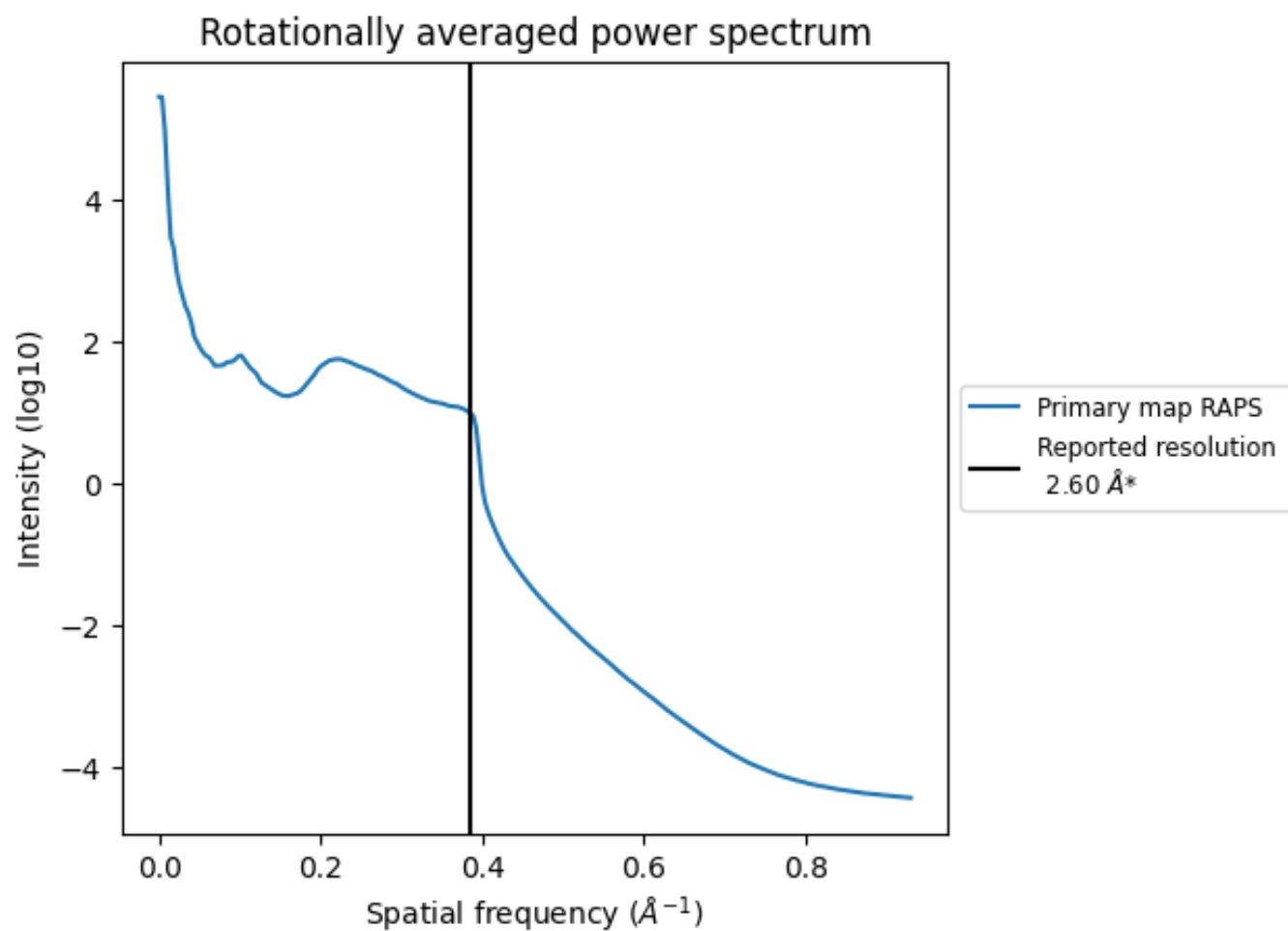
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm³; this corresponds to an approximate mass of 140 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

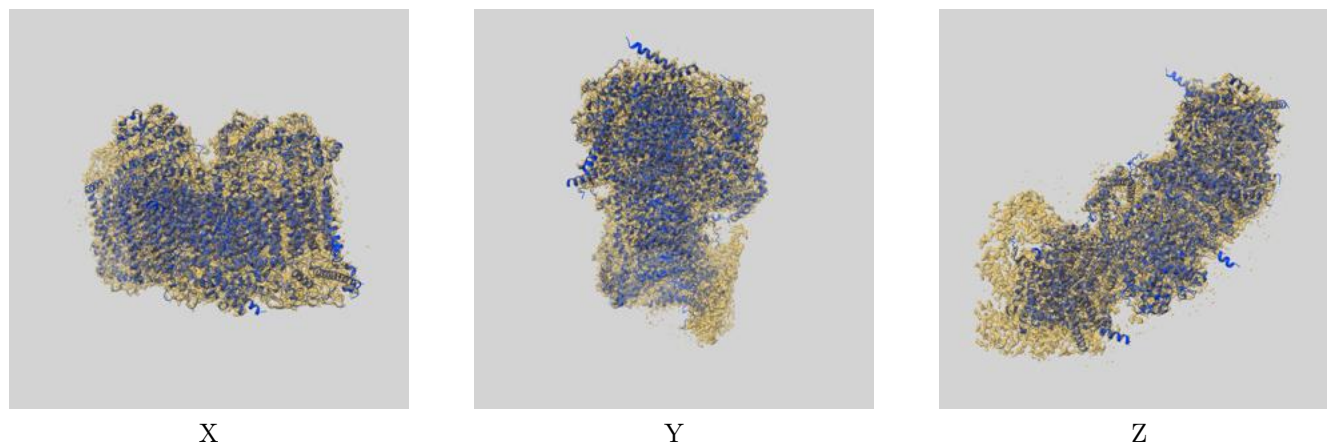
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

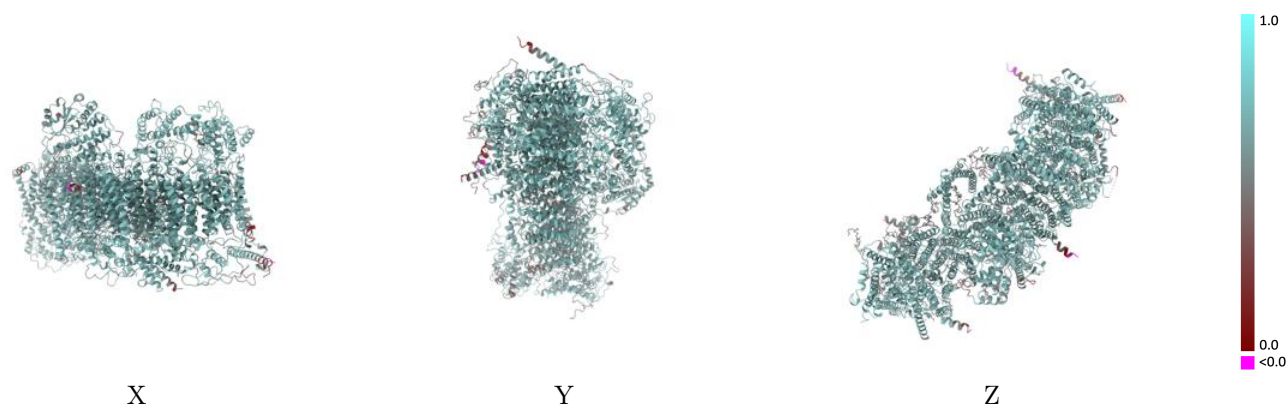
This section contains information regarding the fit between EMDB map EMD-31887 and PDB model 7VC0. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



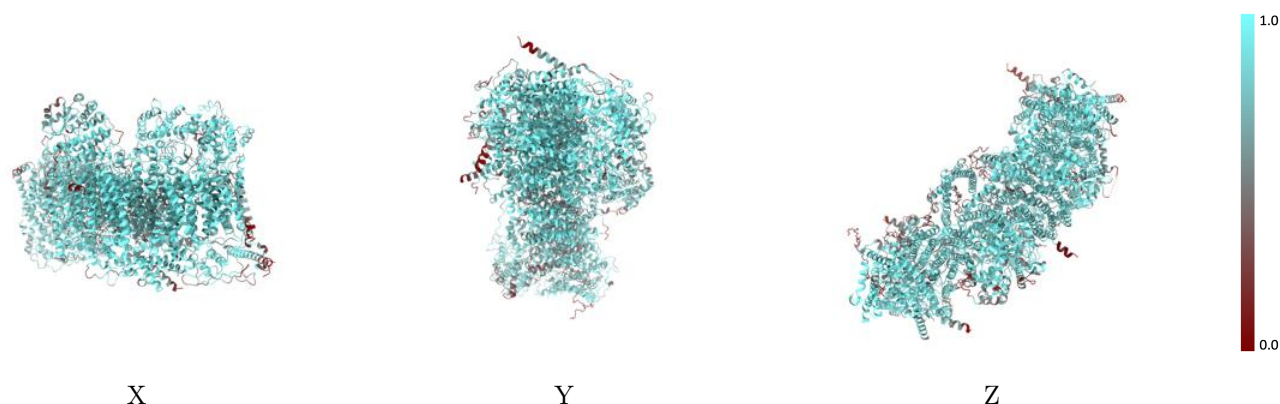
The images above show the 3D surface view of the map at the recommended contour level 0.0152 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



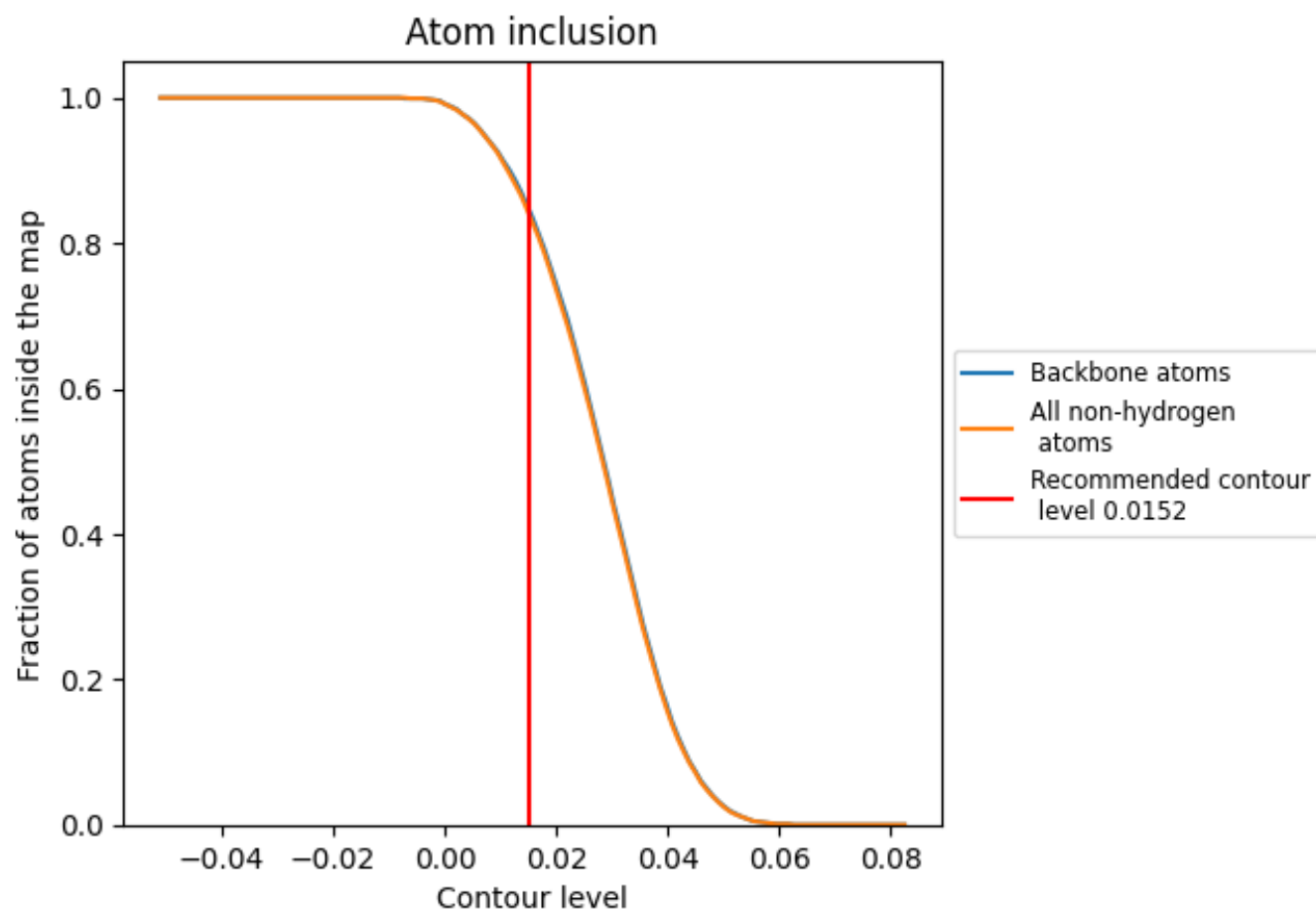
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0152).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.6470
Q	 0.7440	 0.6210
S	 0.8890	 0.6580
U	 0.7560	 0.6100
V	 0.7640	 0.6290
W	 0.8150	 0.6300
X	 0.8220	 0.6480
Y	 0.7220	 0.6050
Z	 0.6750	 0.5700
a	 0.8820	 0.6660
b	 0.7770	 0.6200
c	 0.8630	 0.6570
d	 0.8230	 0.6440
e	 0.7810	 0.6200
f	 0.6400	 0.5690
g	 0.8840	 0.6620
h	 0.7950	 0.6280
i	 0.9540	 0.6910
j	 0.7890	 0.6370
k	 0.8690	 0.6530
l	 0.9040	 0.6750
m	 0.7780	 0.6160
n	 0.6550	 0.5680
o	 0.7970	 0.6380
p	 0.8530	 0.6540
r	 0.9250	 0.6760
s	 0.8970	 0.6670
u	 0.7820	 0.6350
v	 0.7060	 0.5770
w	 0.7790	 0.6260

